SUPPORTING INFORMATION

A_3 and A_2B-fluorocorroles: synthesis, X-ray characterization and antiviral activity evaluation against Human Cytomegalovirus Infection

Sandrine Kappler-Gratias, Léo Bucher, Nicolas Desbois, Yoann Rousselin, Kerstin Bystricky, Claude P. Gros, and Franck Gallardo

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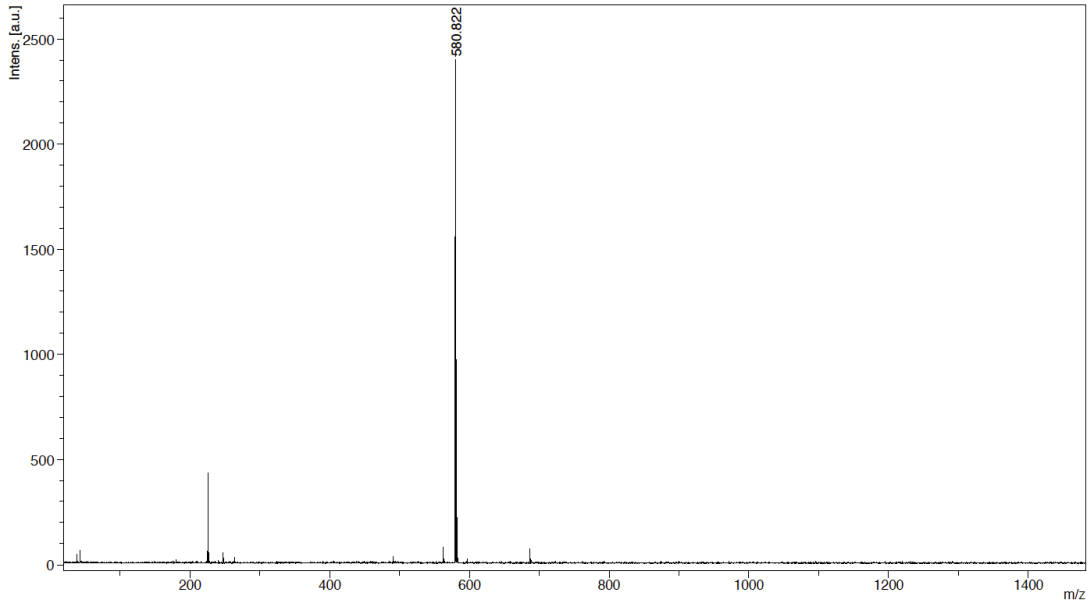
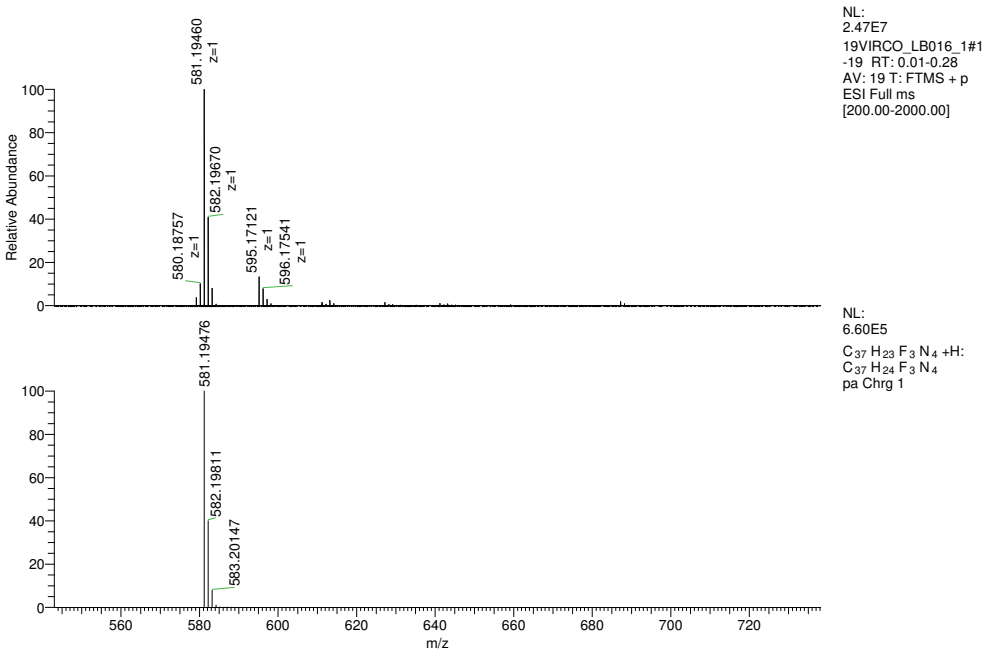
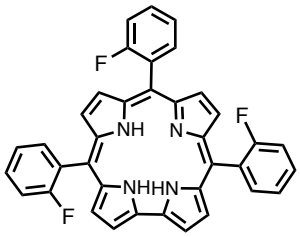






Chemical Formula: $C_{37}H_{23}F_3N_4$

Exact Mass: 580.1875

Molecular Weight: 580.6142

Figure S1: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,10,15-tris(2'-fluorophenyl)corrole **1**.

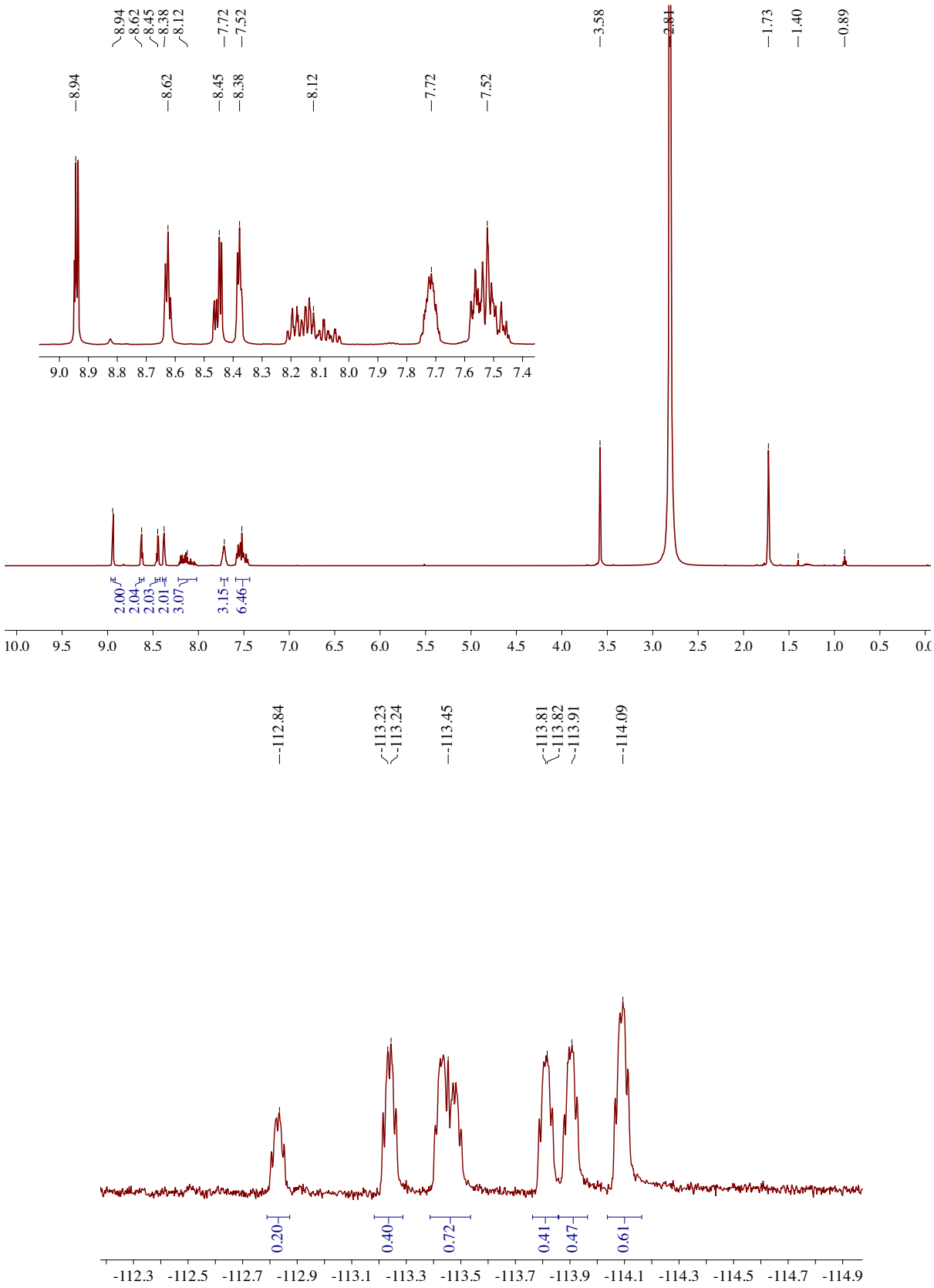


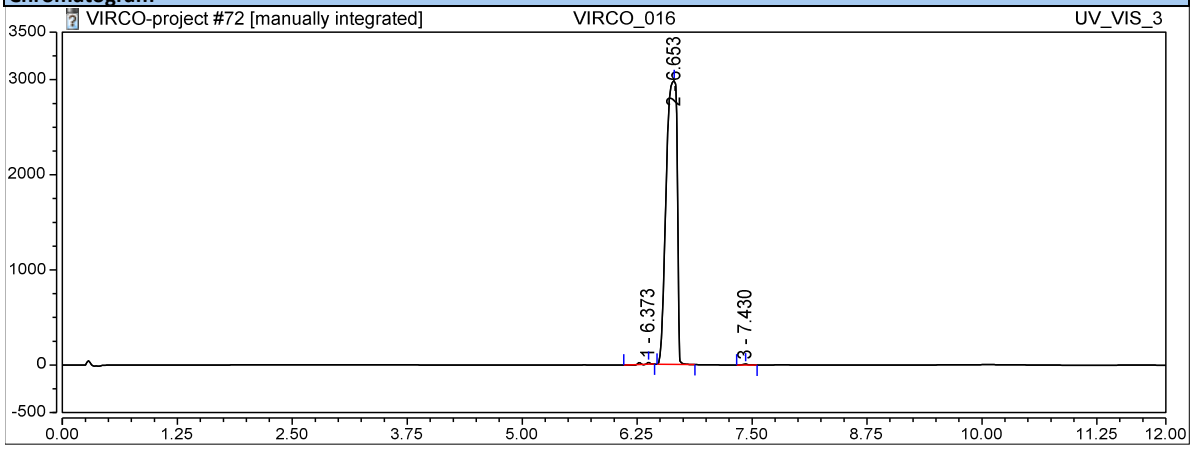
Figure S2: [1]H NMR (top) and [19]F spectra (down) of 5,10,15-tris(2'-fluorophenyl)corrole **1** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

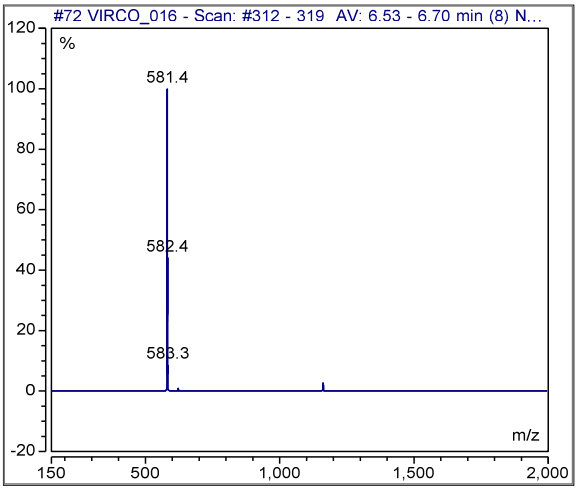
Injection Name:	**VIRCO_016**	*Run Time (min):*	**12.00**
Vial Number:	**RC2**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_3**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**06/Sep/18 18:32**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.373	1.060	19.875	0.26	0.66	n.a.
2		6.653	411.387	2983.970	99.60	99.02	n.a.
3		7.430	0.593	9.575	0.14	0.32	n.a.
Total:			**413.039**	**3013.420**	**100.00**	**100.00**	



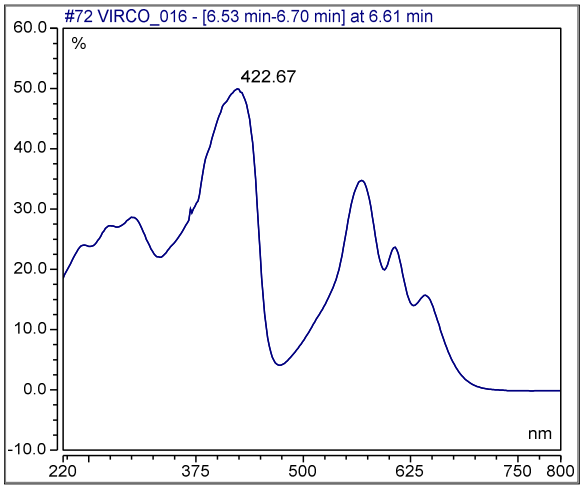
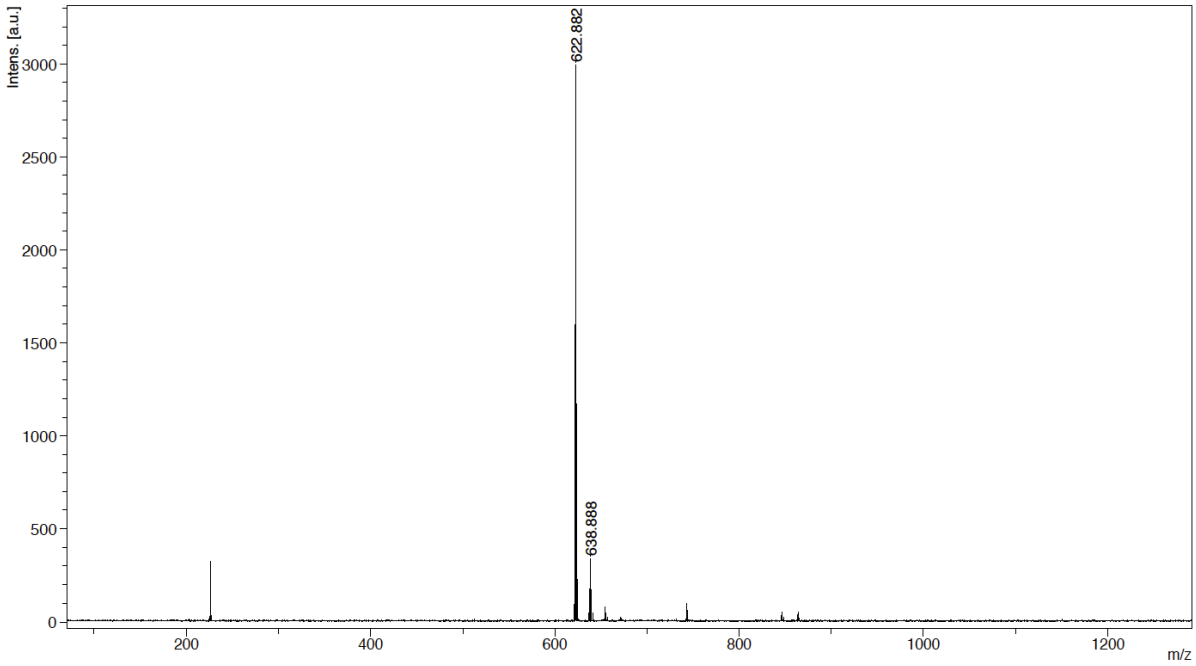
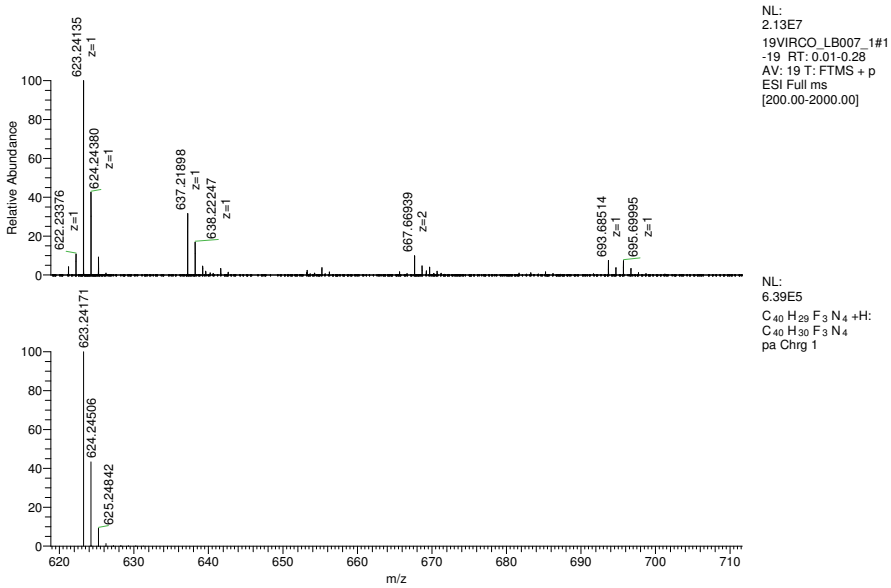
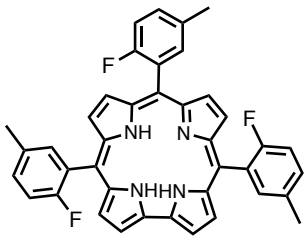


Figure S3: HPLC chromatogram of 5,10,15-tris(2'-fluorophenyl)corrole **1**.







Chemical Formula: $C_{40}H_{29}F_3N_4$
Exact Mass: 622.2344
Molecular Weight: 622.6952

Figure S4: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,10,15-tris(2'-fluoro-5'-methylphenyl)corrole **2**.

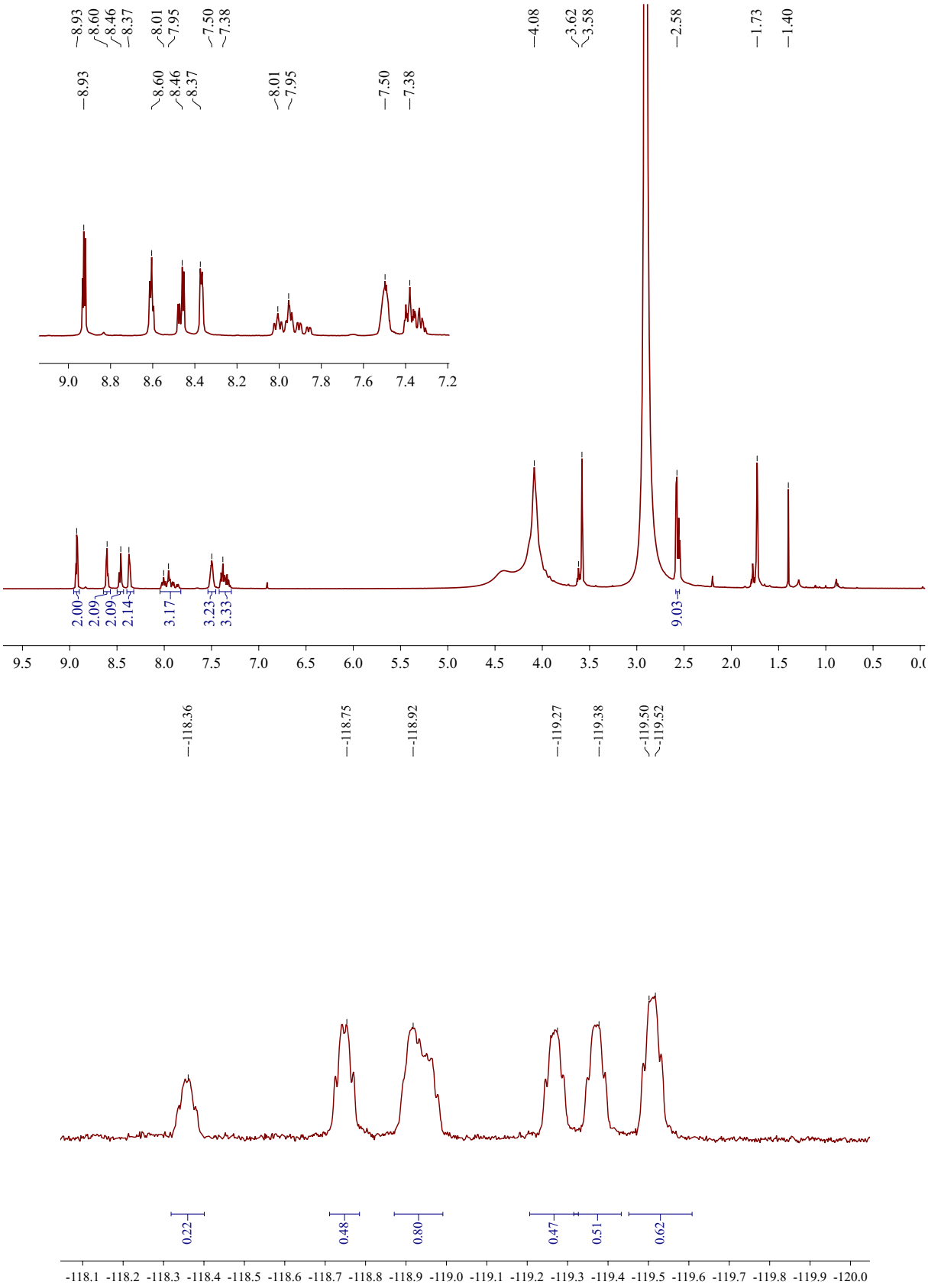


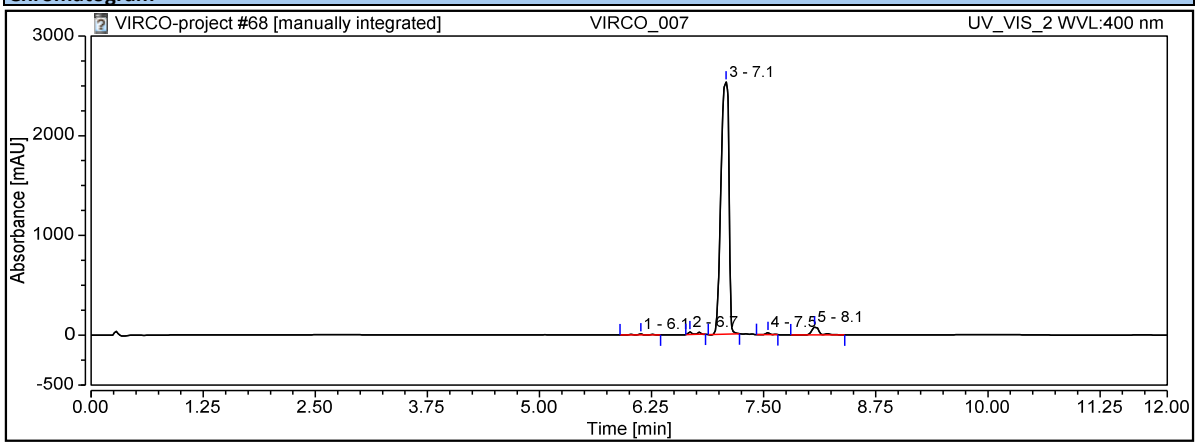
Figure S5: [1]H NMR (top) and [19]F spectra (down) of 5,10,15-tris(2'-fluoro-5'-methylphenyl)corrole **2** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

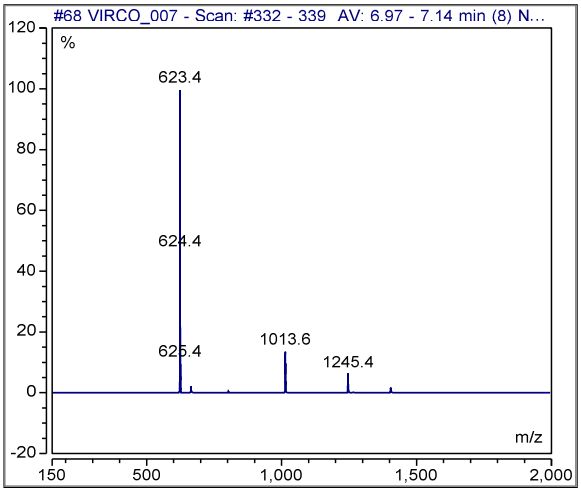
Injection Name:	**VIRCO_007**	*Run Time (min):*	**12.00**
Vial Number:	**BC4**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**06/Sep/18 10:12**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.130	0.988	9.387	0.37	0.35	n.a.
2		6.677	2.093	26.672	0.77	1.00	n.a.
3		7.080	258.876	2528.851	95.74	94.97	n.a.
4		7.547	0.926	19.636	0.34	0.74	n.a.
5		8.067	7.511	78.266	2.78	2.94	n.a.
Total:			**270.394**	**2662.811**	**100.00**	**100.00**	



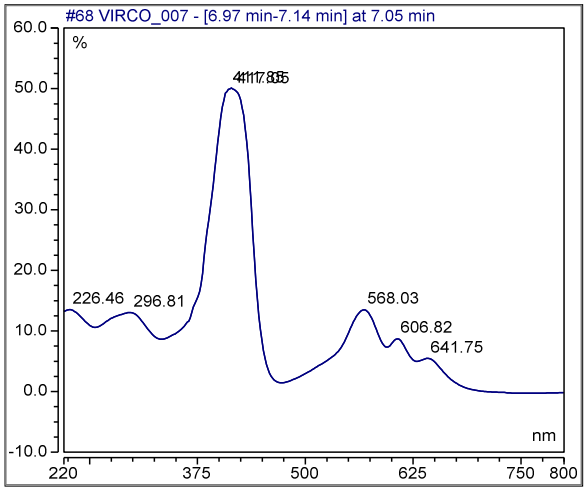
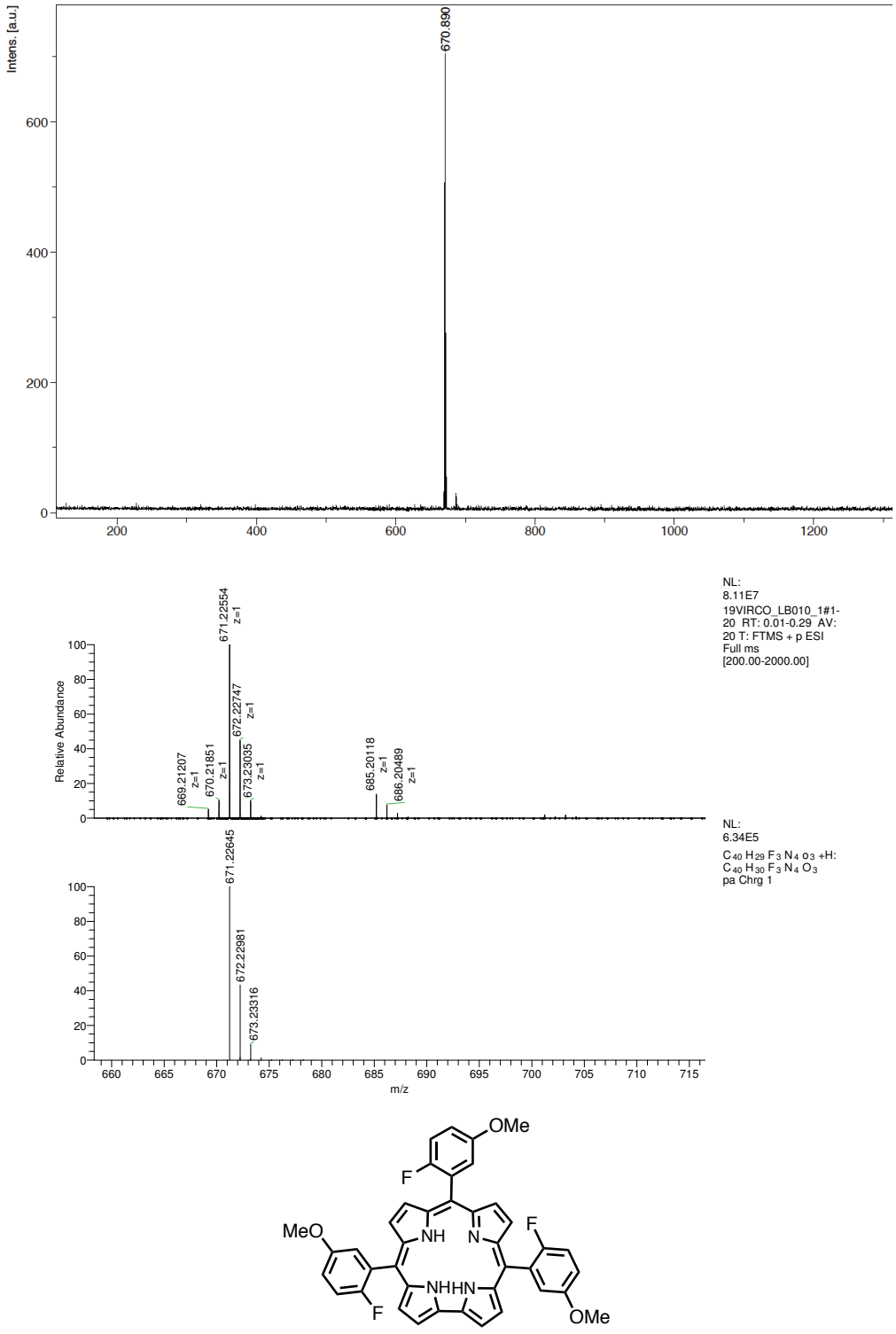


Figure S6: HPLC chromatogram of 5,10,15-tris(2'-fluoro-5'-methylphenyl)corrole **2**.



Chemical Formula: $C_{40}H_{29}F_3N_4O_3$
Exact Mass: 670.2192
Molecular Weight: 670.6922

Figure S7: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,10,15-tris(2'-fluoro-5'-methoxyphenyl)corrole **3**.

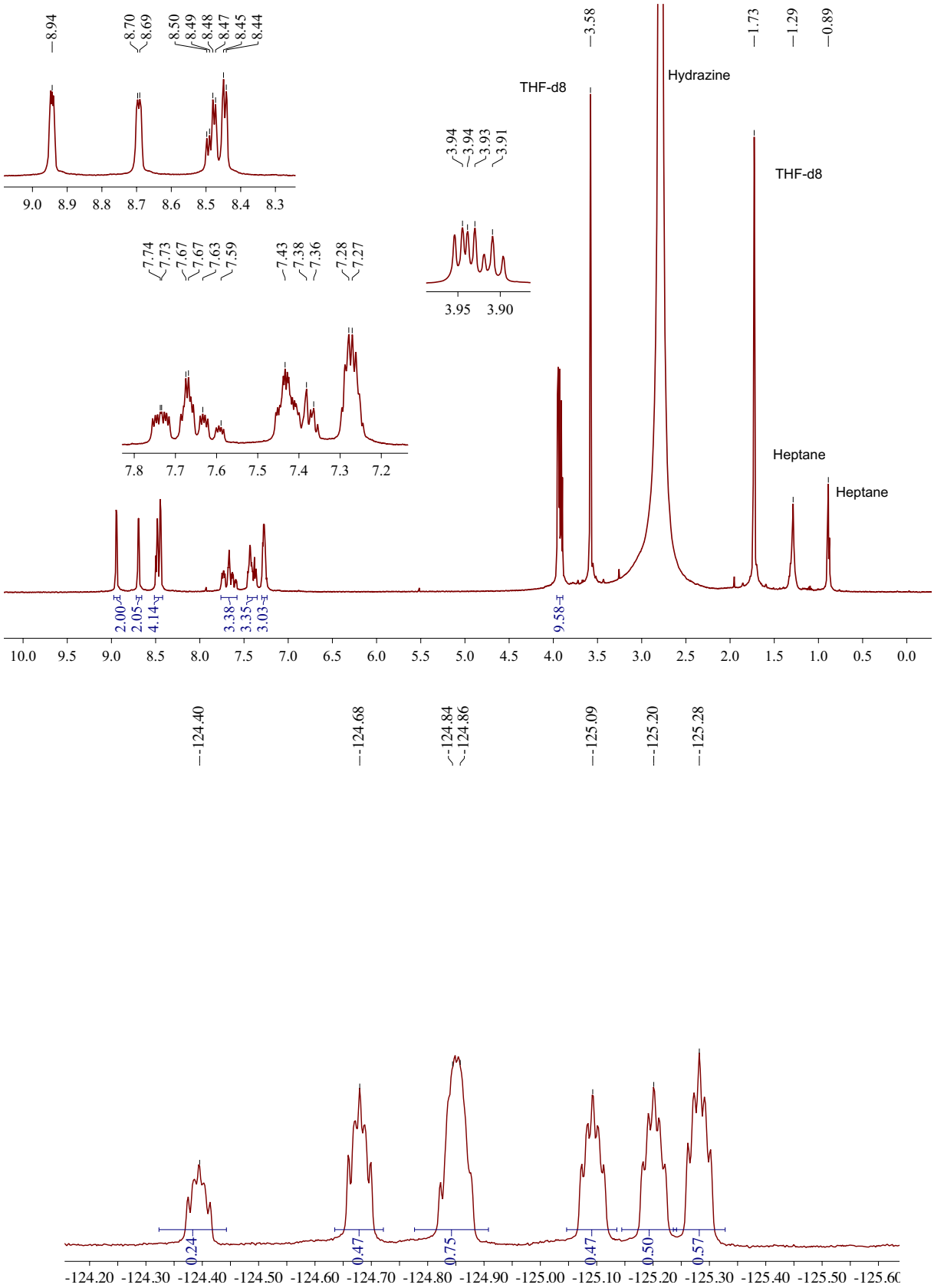


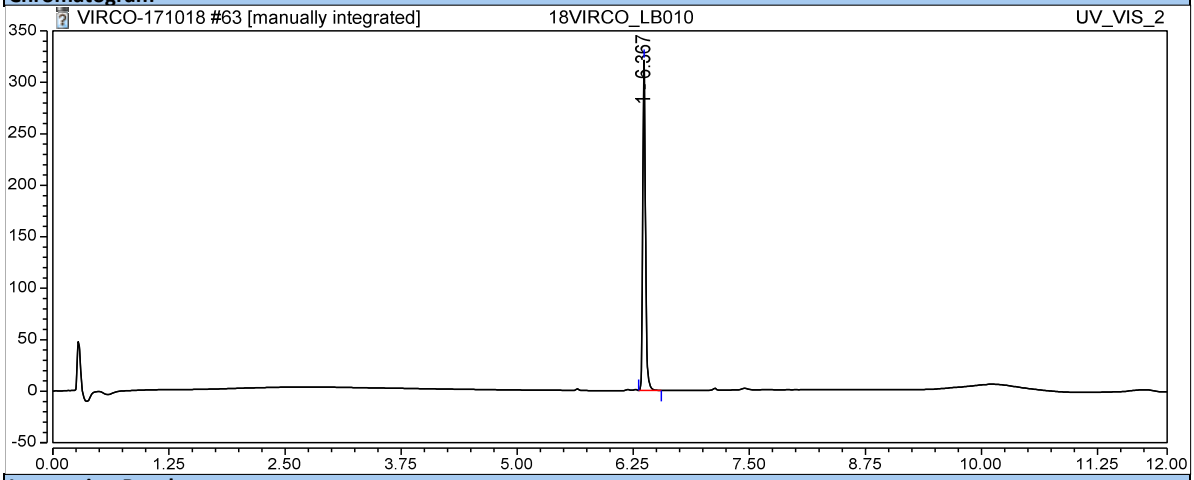
Figure S8: ^{1}H NMR (top) and ^{19}F spectra (down) of 5,10,15-tris(2'-fluoro-5'-methoxyphenyl)corrole **3** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

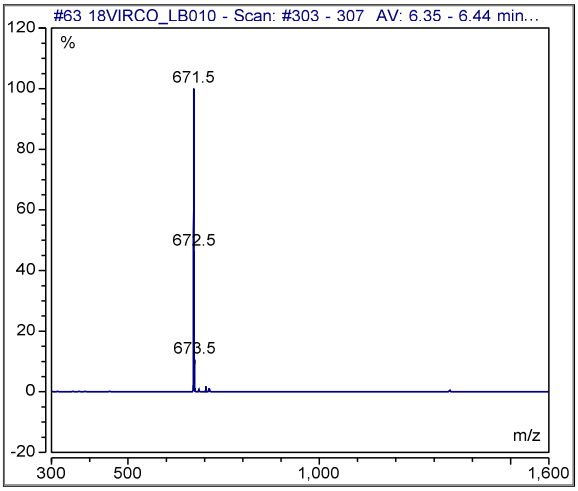
Injection Name:	**18VIRCO_LB010**	*Run Time (min):*	**12.00**
Vial Number:	**GD5**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**18/Apr/19 20:31**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.367	11.048	320.727	100.00	100.00	n.a.
Total:			**11.048**	**320.727**	**100.00**	**100.00**	



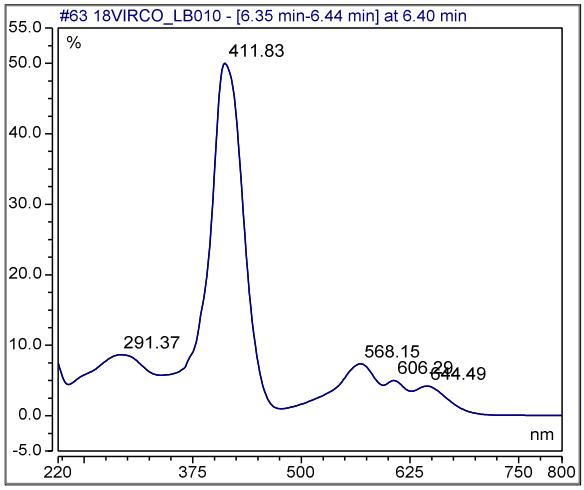
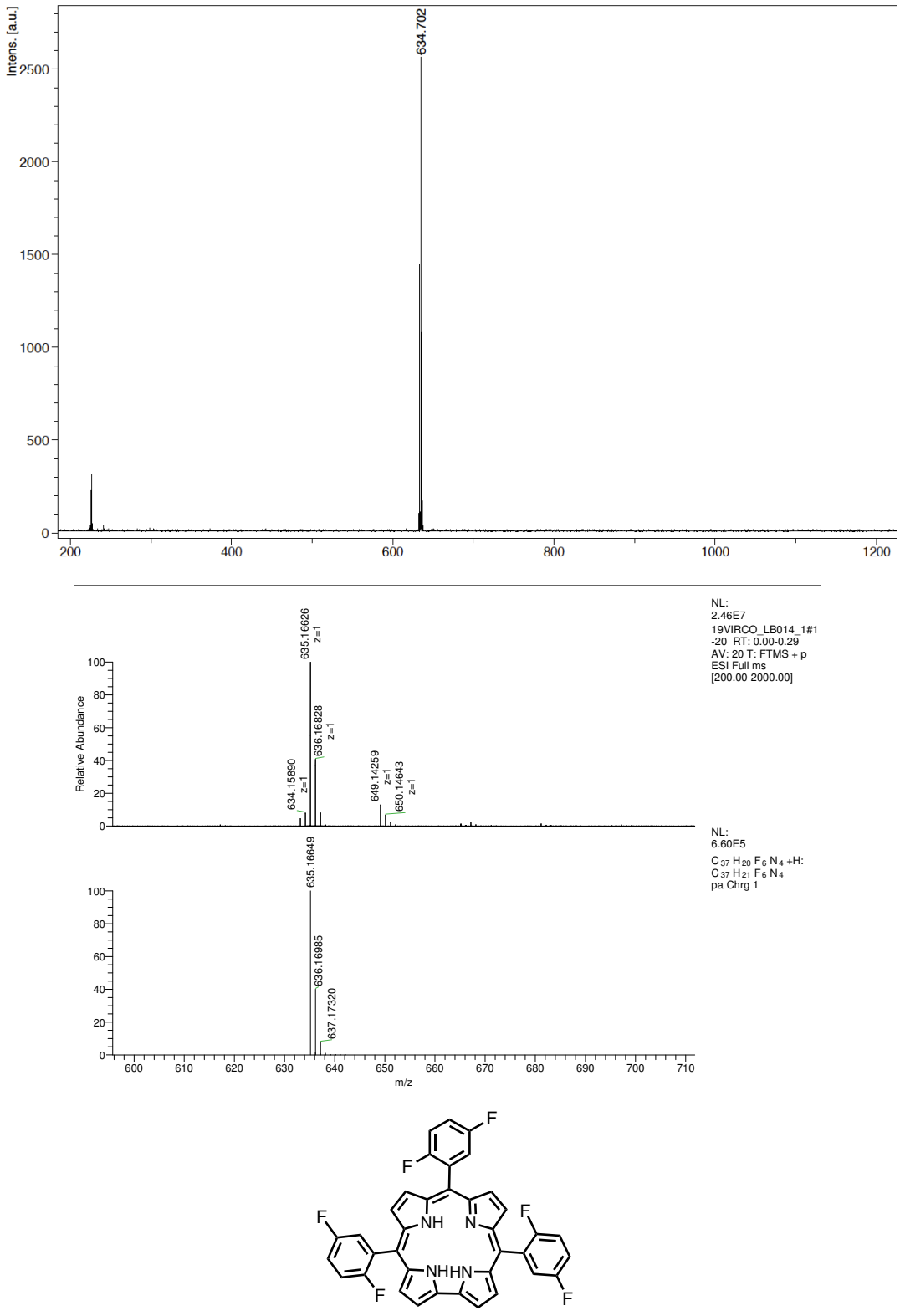


Figure S9: HPLC chromatogram of 5,10,15-tris(2'-fluoro-5'-methoxyphenyl)corrole **3**.



Chemical Formula: $C_{37}H_{20}F_6N_4$
Exact Mass: 634.1592
Molecular Weight: 634.5854

Figure S10: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,10,15-tris(2',5'-difluorophenyl)corrole **4**.

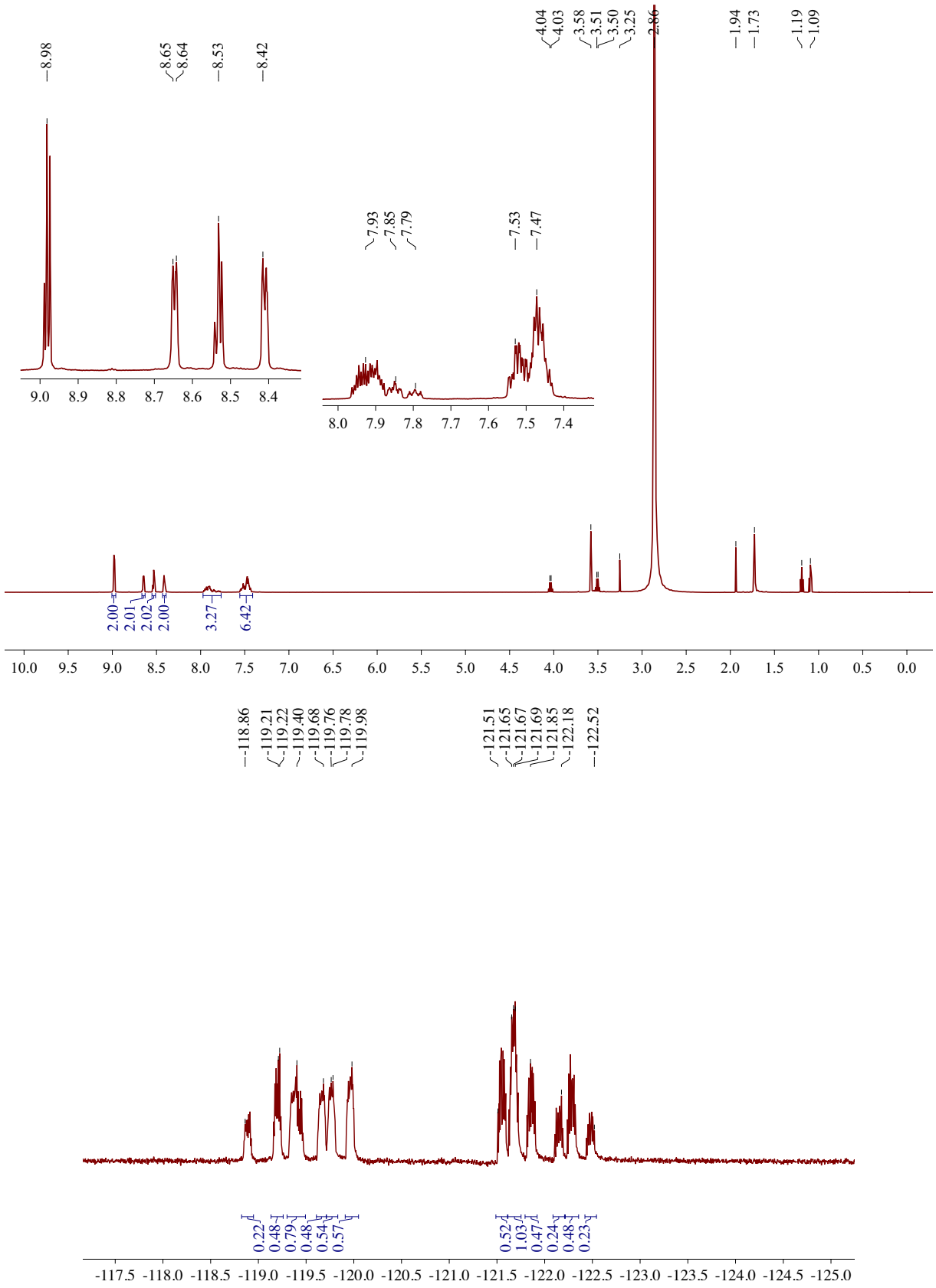


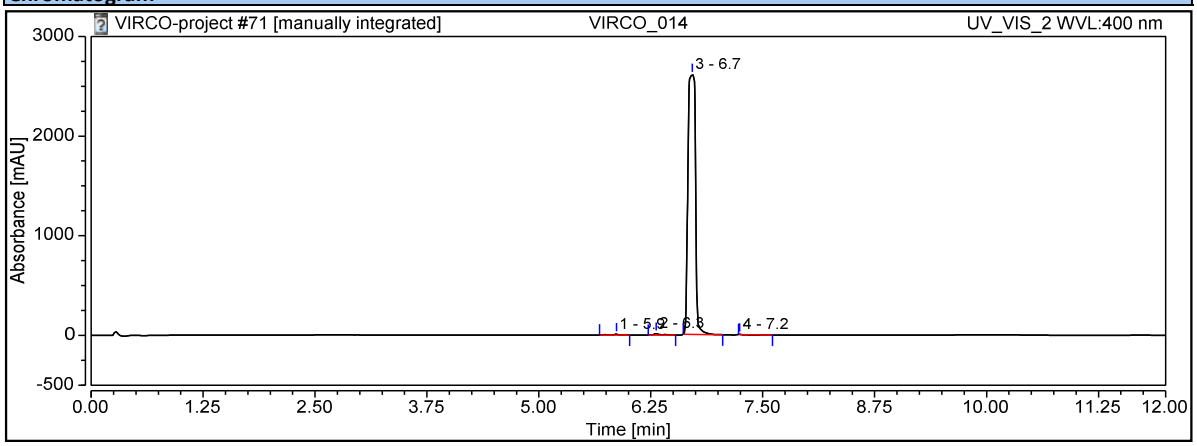
Figure S11: [1]H NMR (top) and [19]F spectra (down) of 5,10,15-tris(2',5'-difluorophenyl)corrole **4** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

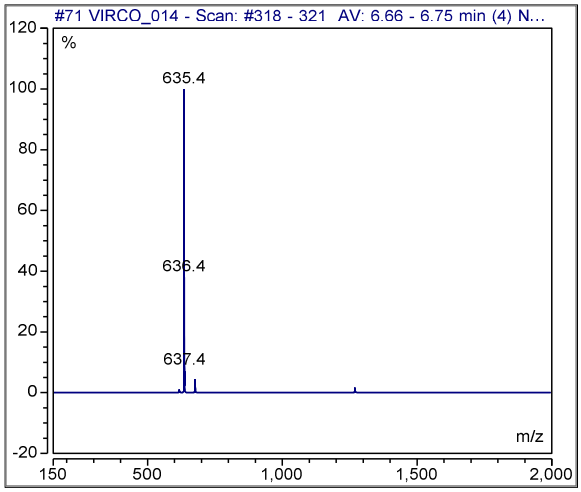
Injection Name:	**VIRCO_014**	*Run Time (min):*	**12.00**
Vial Number:	**RC1**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**06/Sep/18 18:19**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.867	0.571	10.546	0.22	0.40	n.a.
2		6.310	1.444	19.006	0.56	0.72	n.a.
3		6.713	253.176	2609.544	99.03	98.80	n.a.
4		7.243	0.472	2.070	0.18	0.08	n.a.
Total:			**255.663**	**2641.167**	**100.00**	**100.00**	



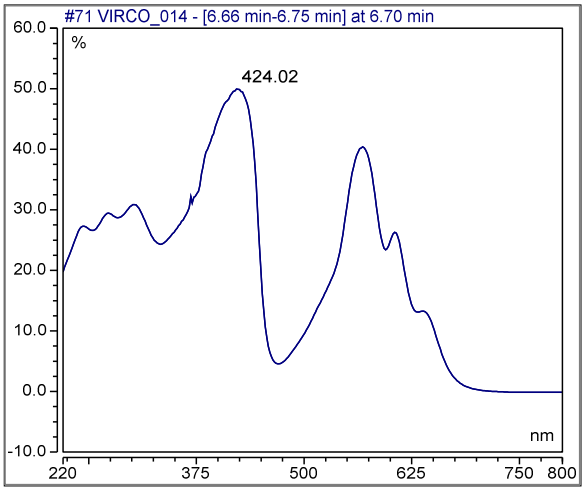
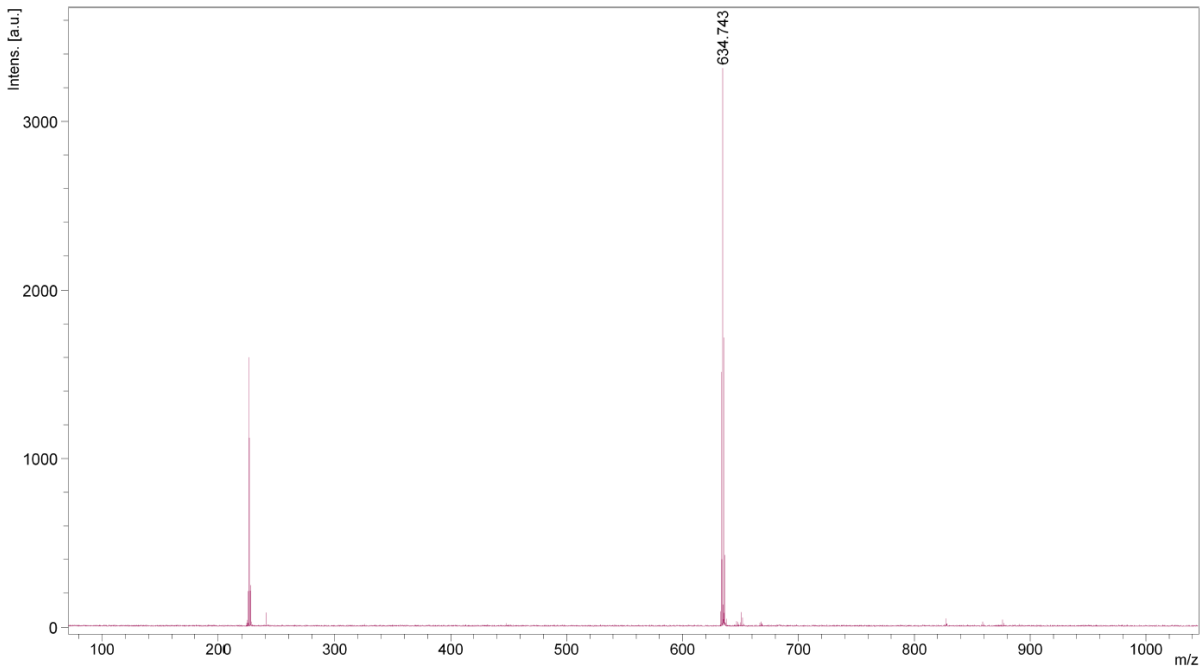
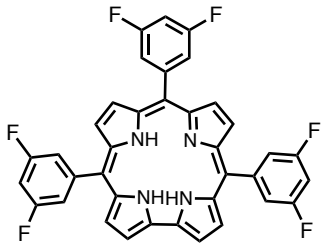


Figure S12: HPLC chromatogram of 5,10,15-tris(2',5'-difluorophenyl)corrole **4**.





Chemical Formula: $C_{37}H_{20}F_6N_4$
Exact Mass: 634.1592
Molecular Weight: 634.5854

Figure S13: MALDI/TOF LRMS mass spectrum of 5,10,15-tris(3',5'-difluorophenyl)corrole **5**.

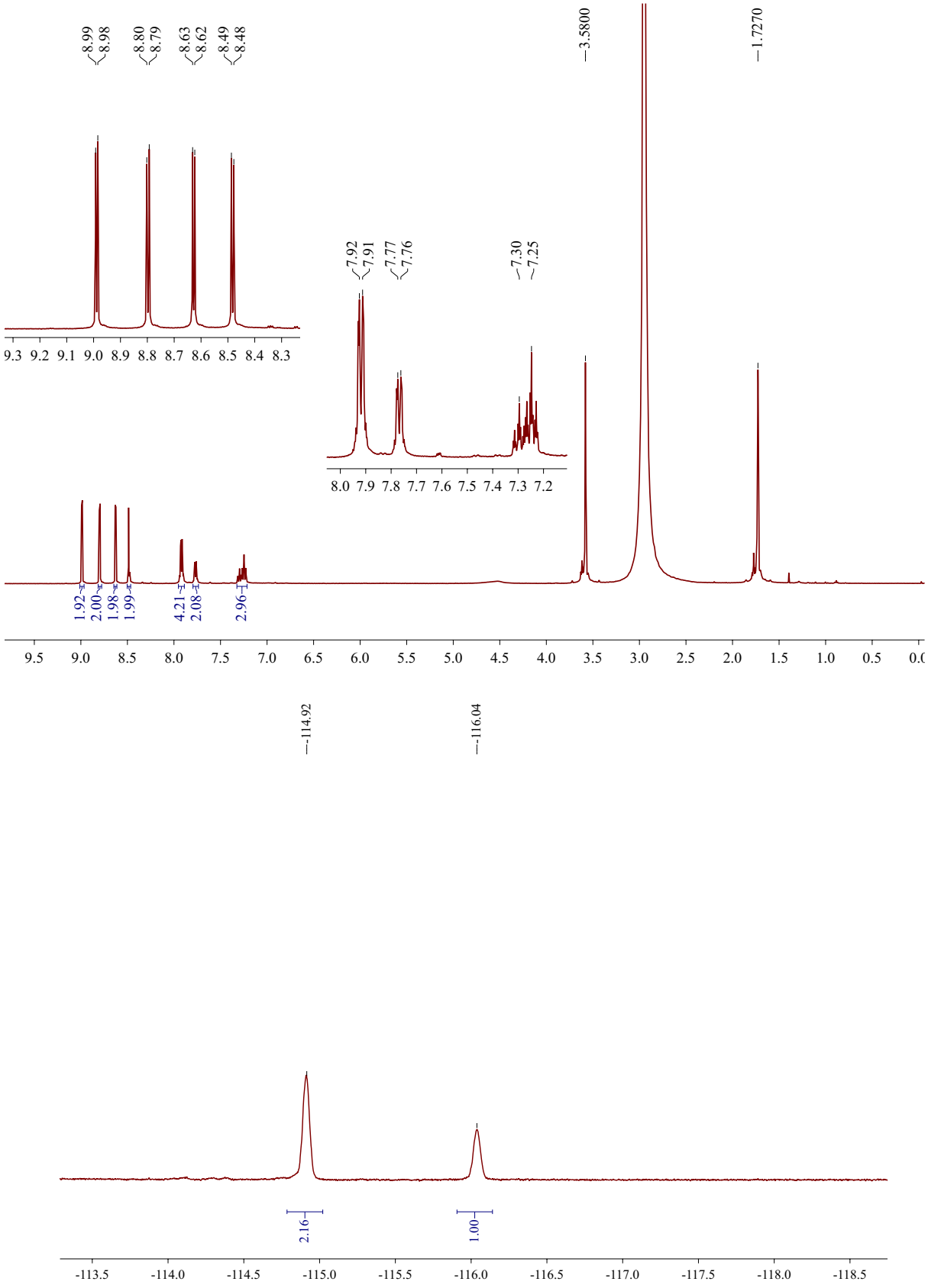


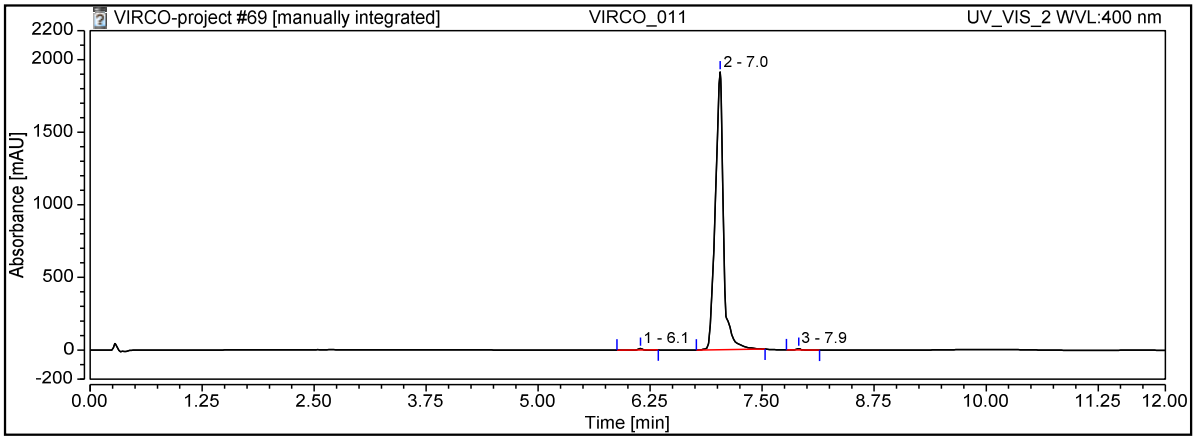
Figure S14: [1]H NMR (top) and [19]F spectra (down) of 5,10,15-tris(3',5'-difluorophenyl)corrole **5** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

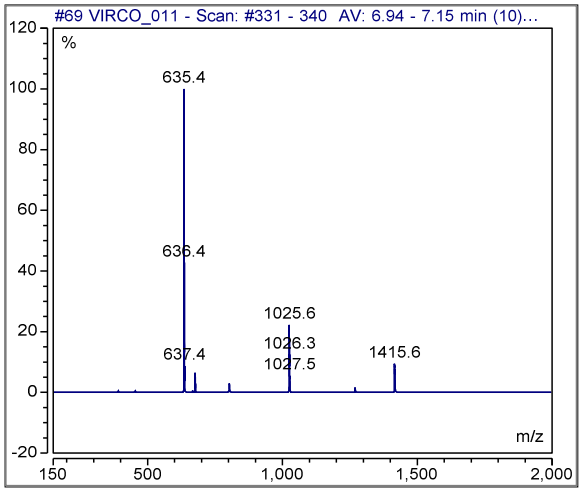
Injection Name:	**VIRCO_011**	*Run Time (min):*	**12.00**
Vial Number:	**BC5**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**06/Sep/18 10:25**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.143	0.571	11.310	0.28	0.58	n.a.
2		7.030	203.052	1913.624	99.50	98.90	n.a.
3		7.907	0.449	9.938	0.22	0.51	n.a.
Total:			**204.072**	**1934.873**	**100.00**	**100.00**	



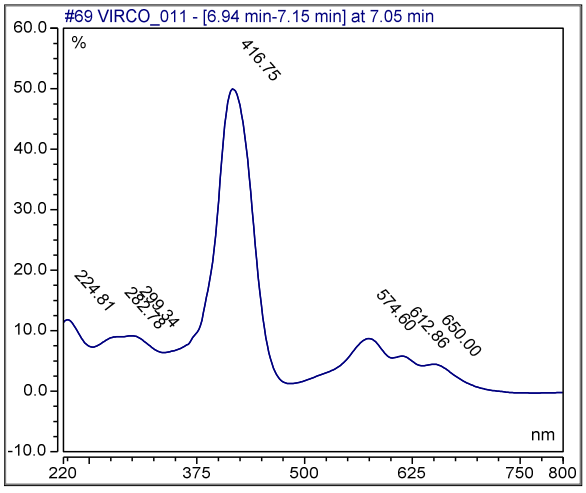
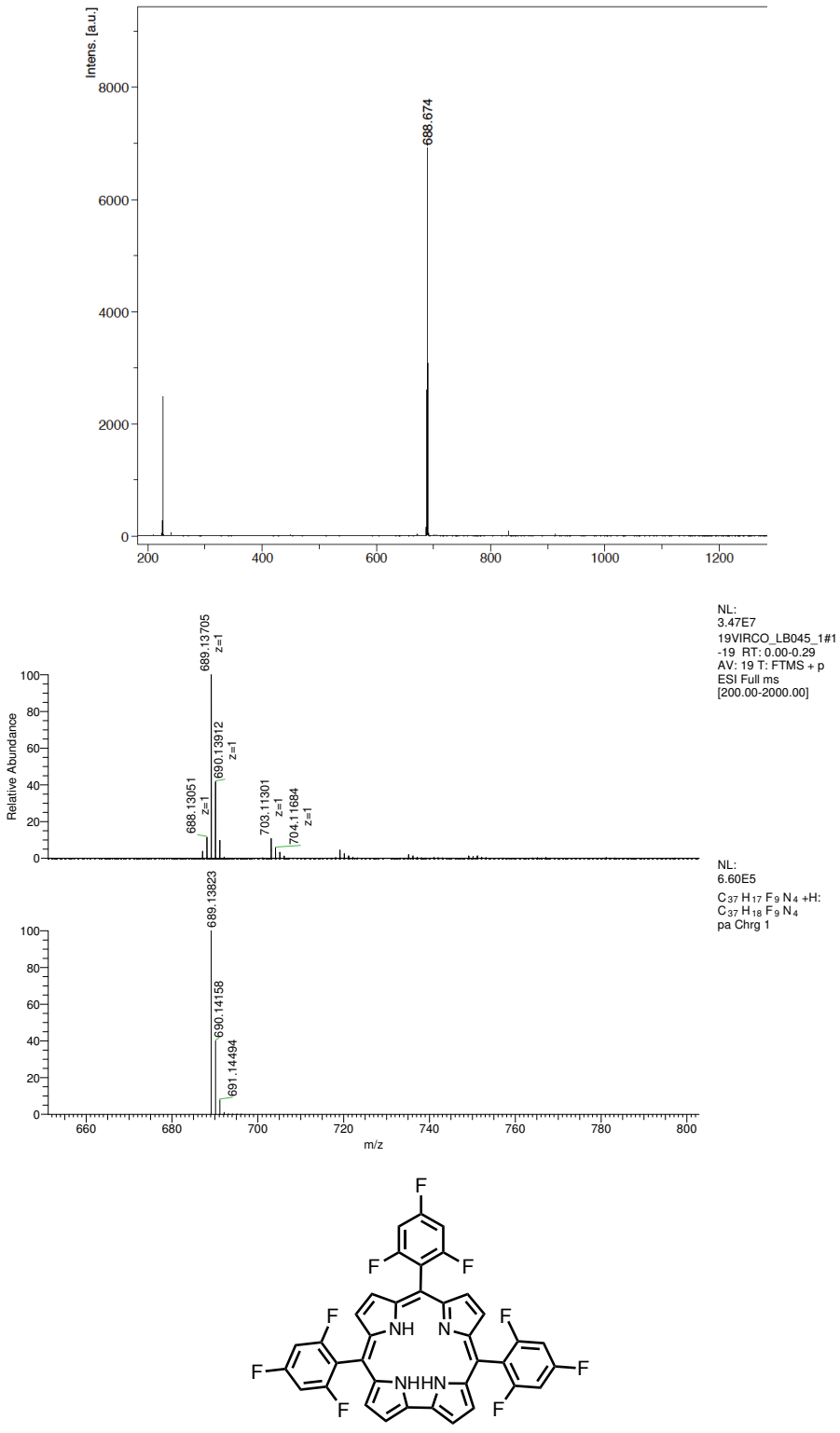


Figure S15: HPLC chromatogram of 5,10,15-tris(3',5'-difluorophenyl)corrole **5**.



Chemical Formula: $C_{37}H_{17}F_9N_4$
Exact Mass: 688.1310
Molecular Weight: 688.5566

Figure S16: MALDI/TOF LRMS and ESI HRMS mass spectrum of 5,10,15-tris(2',4',6'-trifluorophenyl)corrole **6**.

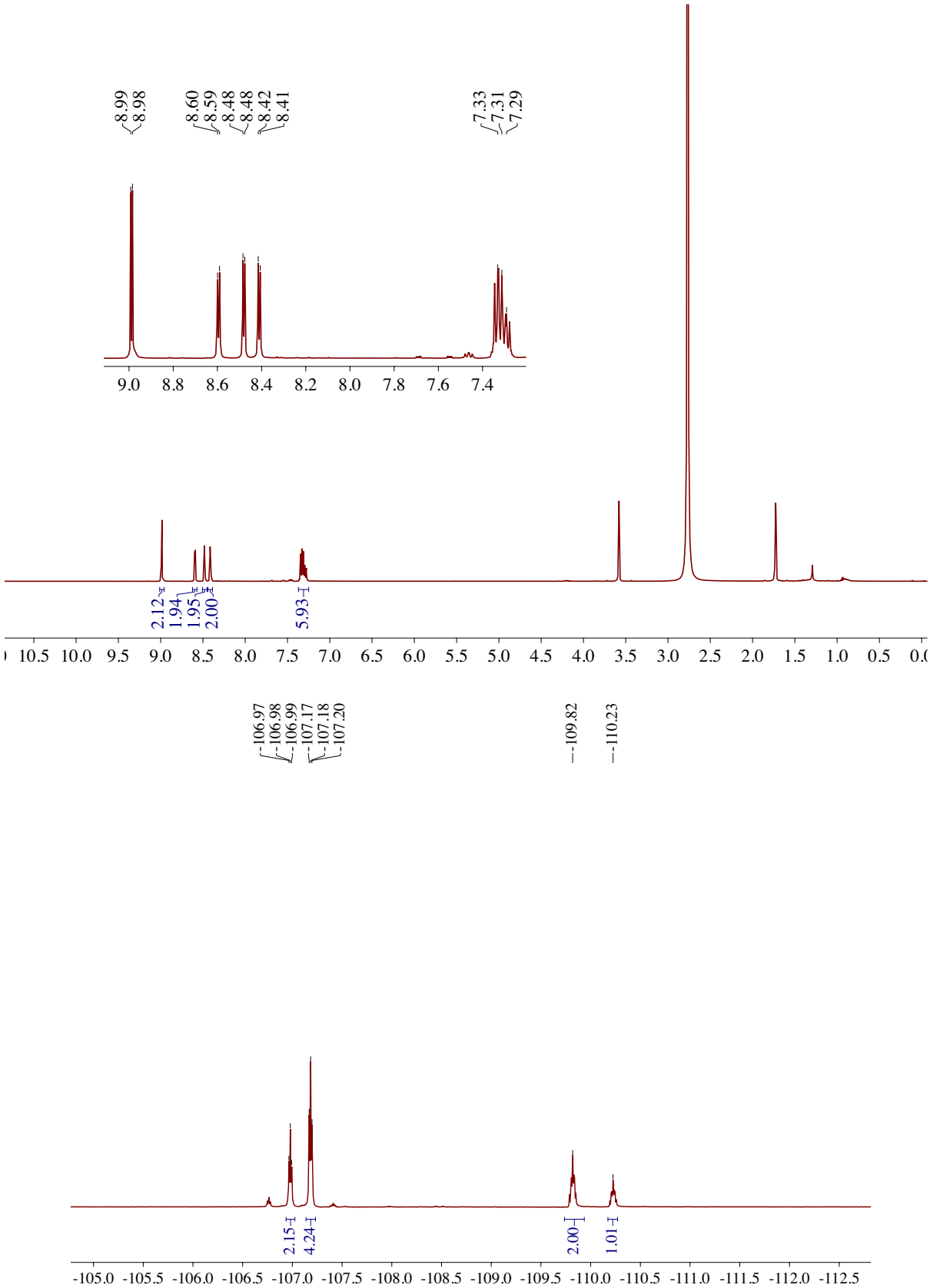


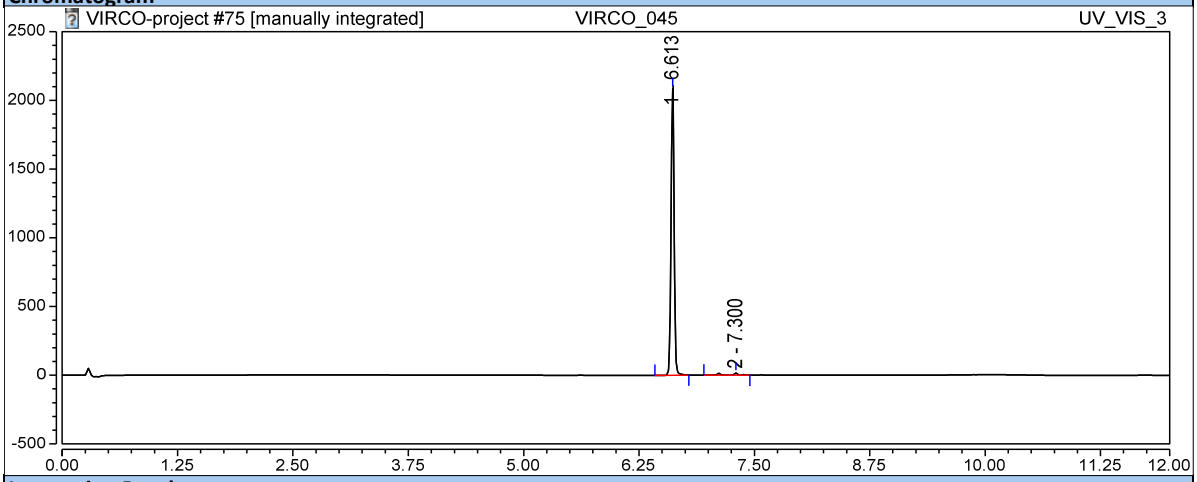
Figure S17: [1]H NMR (top) and [19]F spectra (down) of 5,10,15-tris(2',4',6'-trifluorophenyl)corrole **6** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

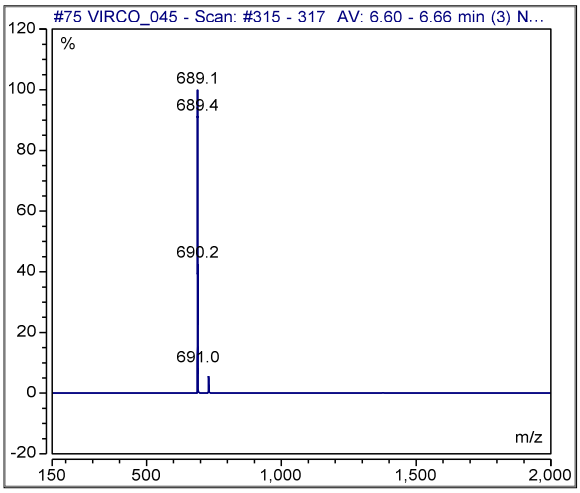
Injection Name:	**VIRCO_045**	*Run Time (min):*	**12.00**
Vial Number:	**RD3**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_3**
Calibration Level:		*Wavelength:*	**440**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**07/Sep/18 14:52**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.613	82.440	2084.331	98.76	99.27	n.a.
2		7.300	1.037	15.412	1.24	0.73	n.a.
Total:			**83.477**	**2099.744**	**100.00**	**100.00**	



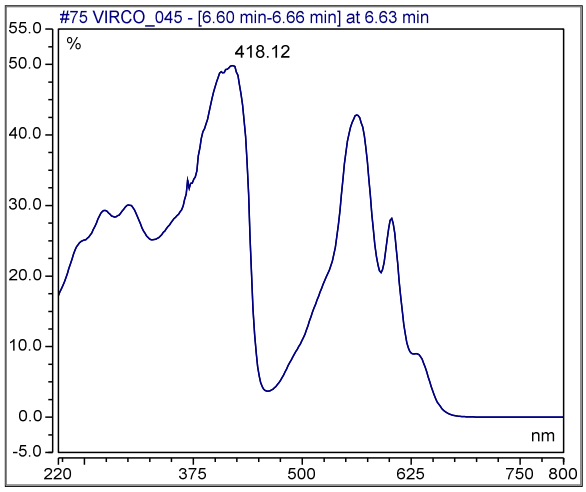
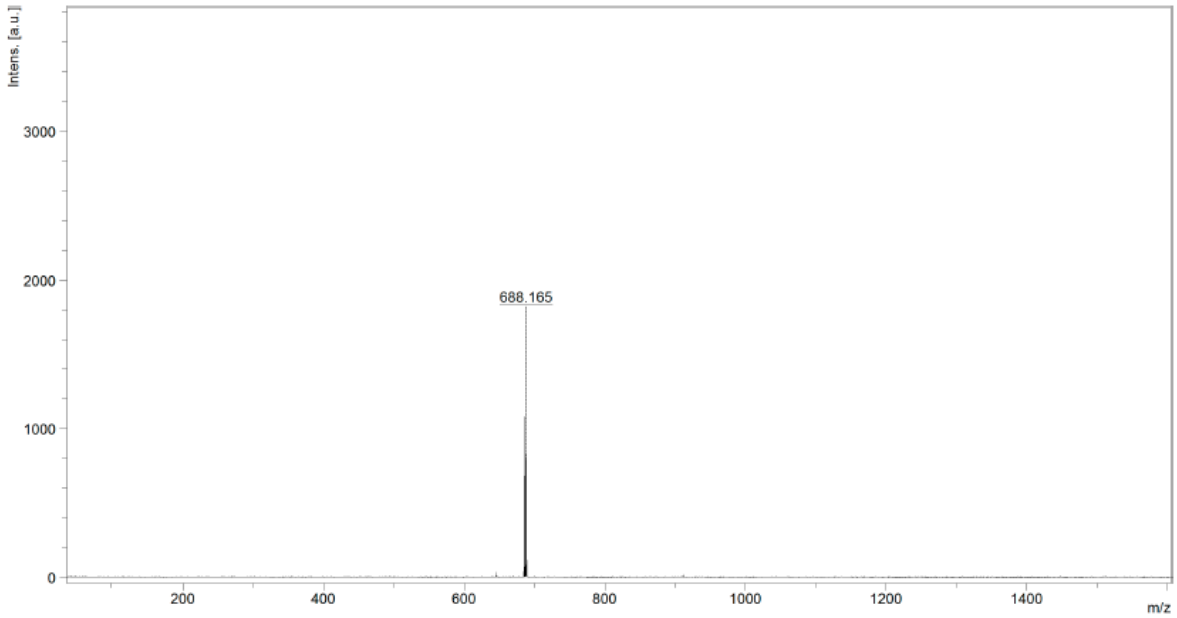
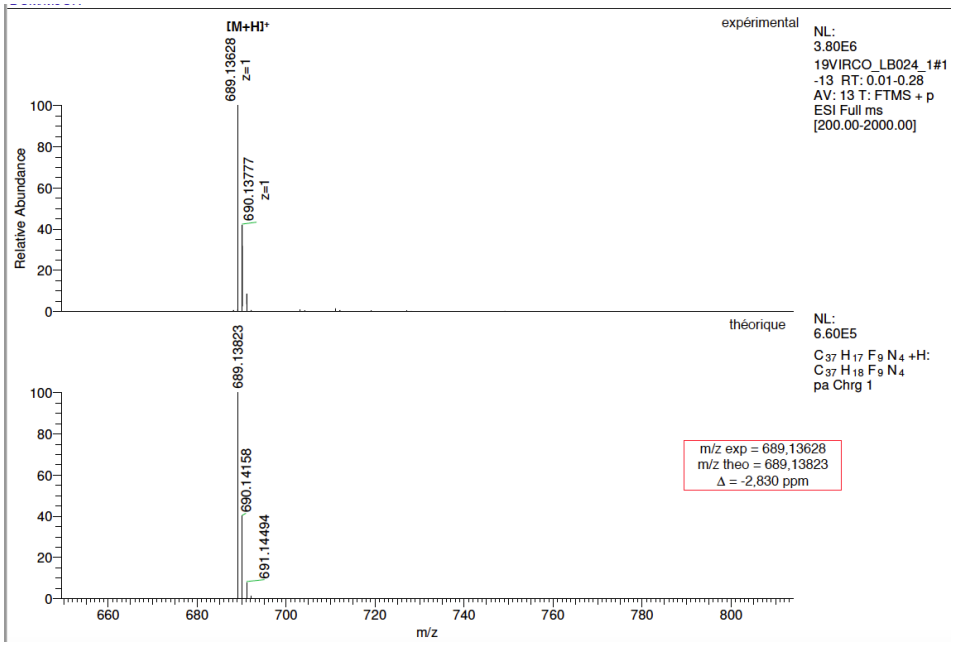
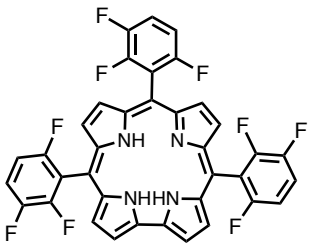


Figure S18: HPLC chromatogram of 5,10,15-tris(2',4',6'-trifluorophenyl)corrole **6**.







Chemical Formula: $C_{37}H_{17}F_9N_4$
Exact Mass: 688.1310
Molecular Weight: 688.5566

Figure S19: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,10,15-tris(2',3',6'-trifluorophenyl)corrole **7**.

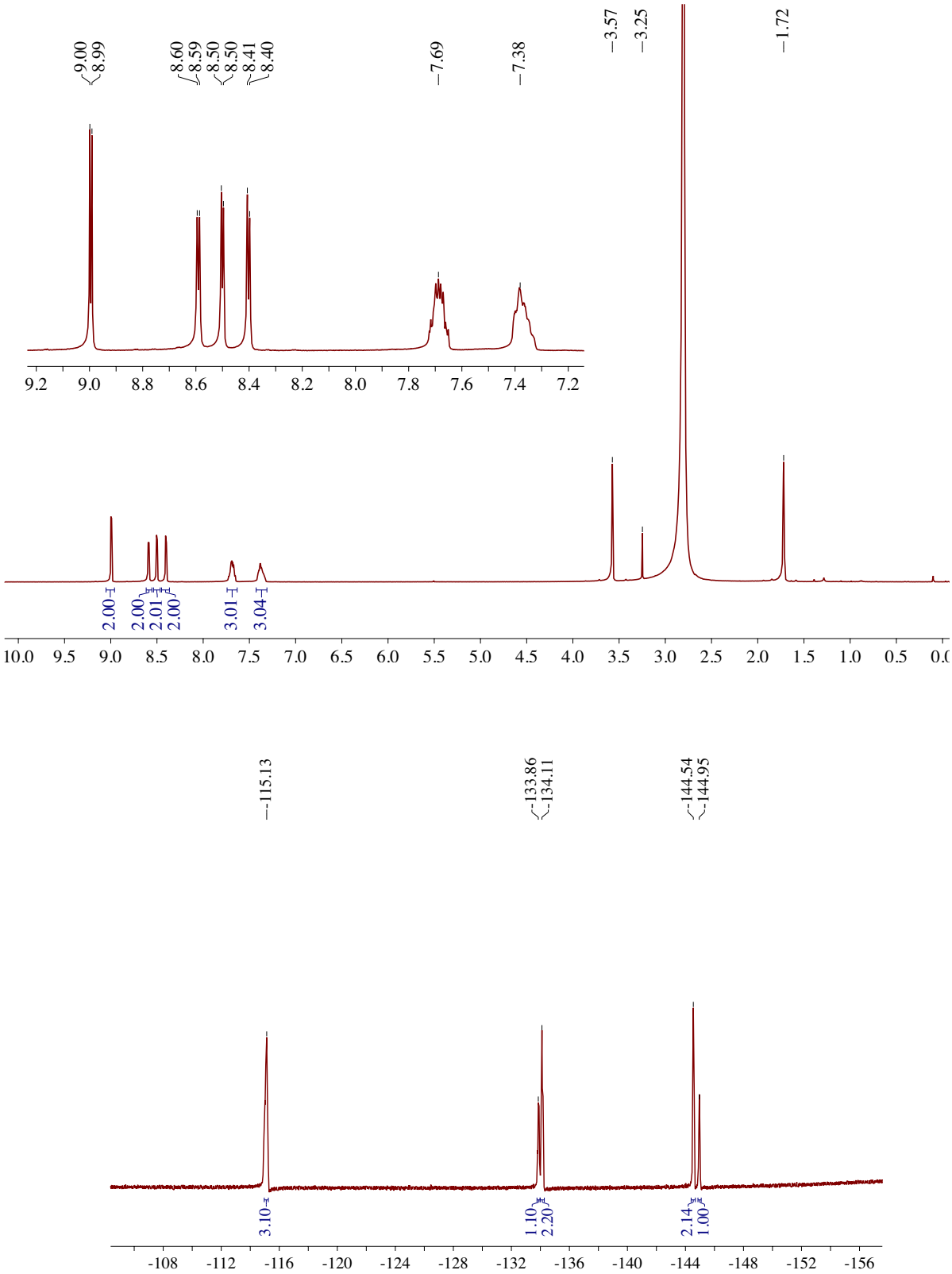


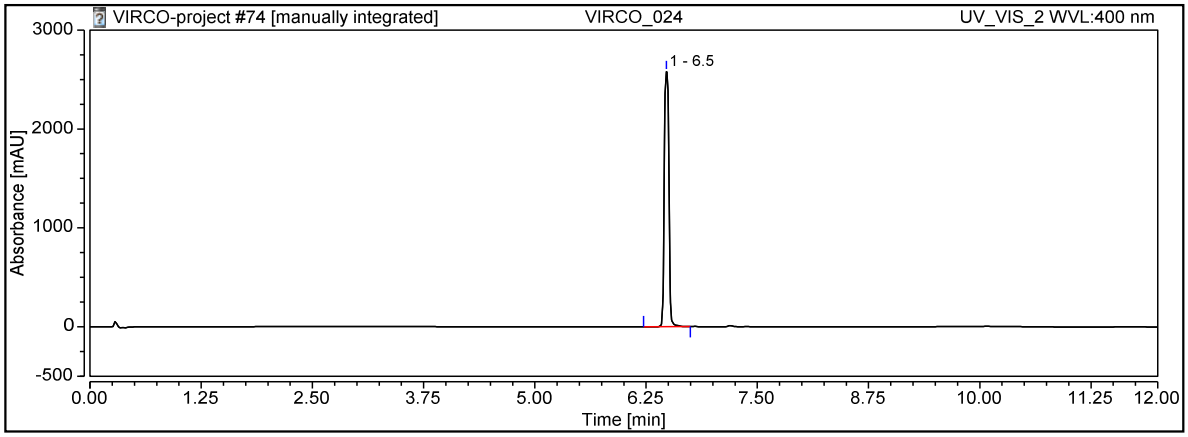
Figure S20: [1]H NMR (top) and [19]F spectra (down) of 5,10,15-tris(2',3',6'-trifluorophenyl)corrole **7** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

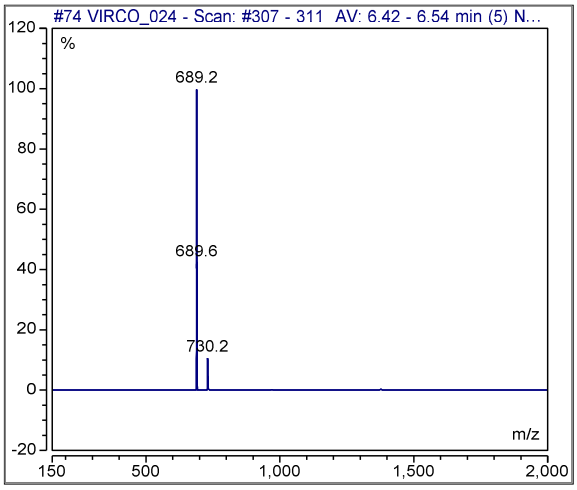
Injection Name:	**VIRCO_024**	*Run Time (min):*	**12.00**
Vial Number:	**RD2**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**07/Sep/18 14:38**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.477	155.203	2579.229	100.00	100.00	n.a.
Total:			**155.203**	**2579.229**	**100.00**	**100.00**	



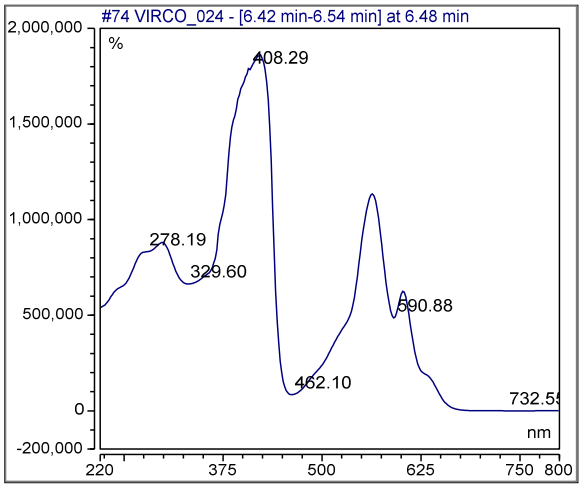
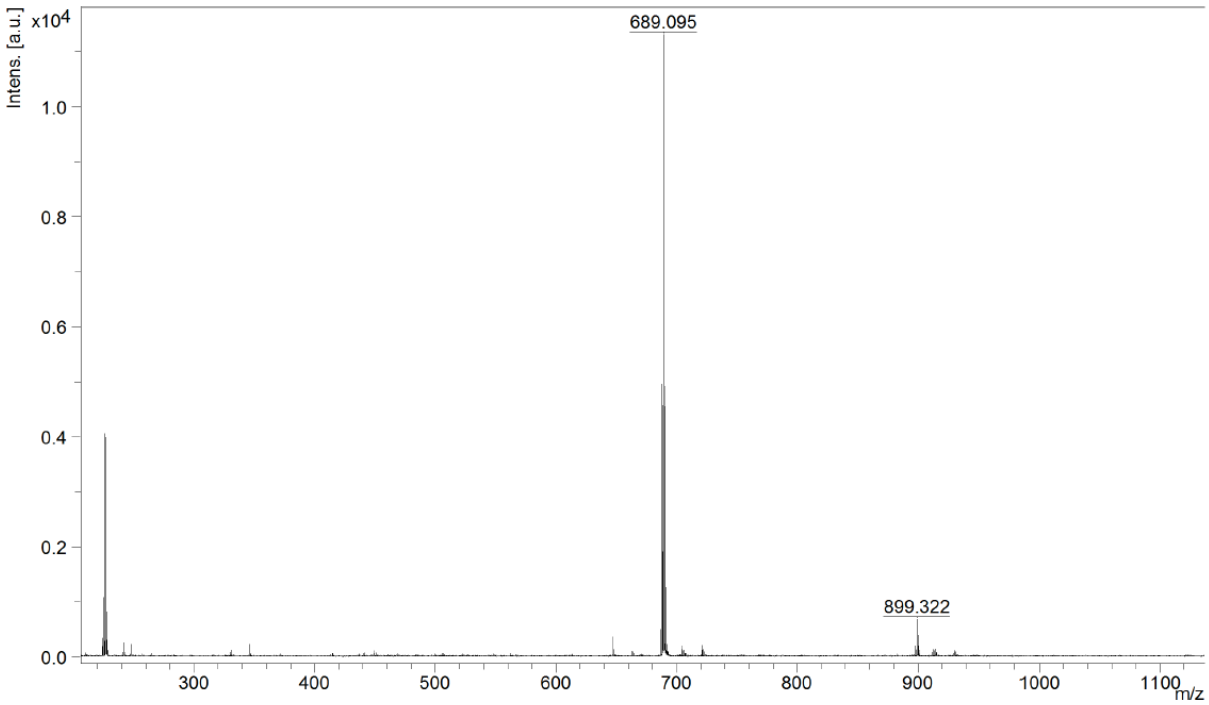
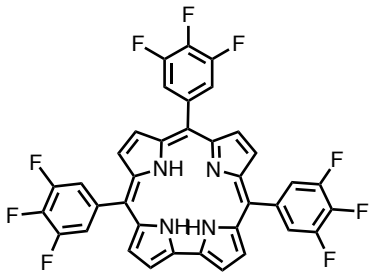


Figure S21: HPLC chromatogram of 5,10,15-tris(2',3',6'-trifluorophenyl)corrole **7**.





Chemical Formula: $C_{37}H_{17}F_9N_4$
Exact Mass: 688.1310
Molecular Weight: 688.5566

Figure S22: MALDI/TOF mass spectrum of 5,10,15-tris(3',4',5'-trifluorophenyl)corrole **8**.

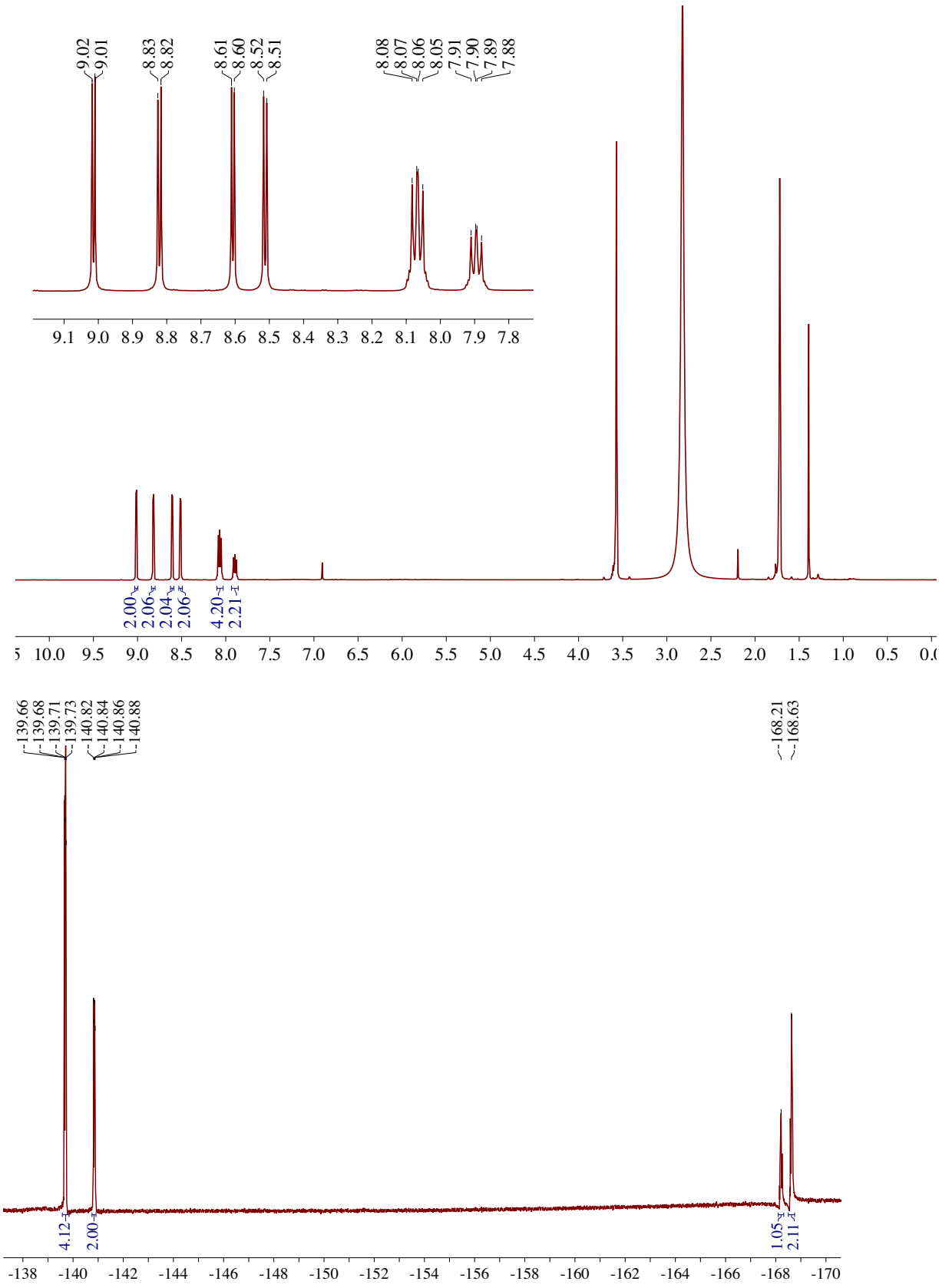


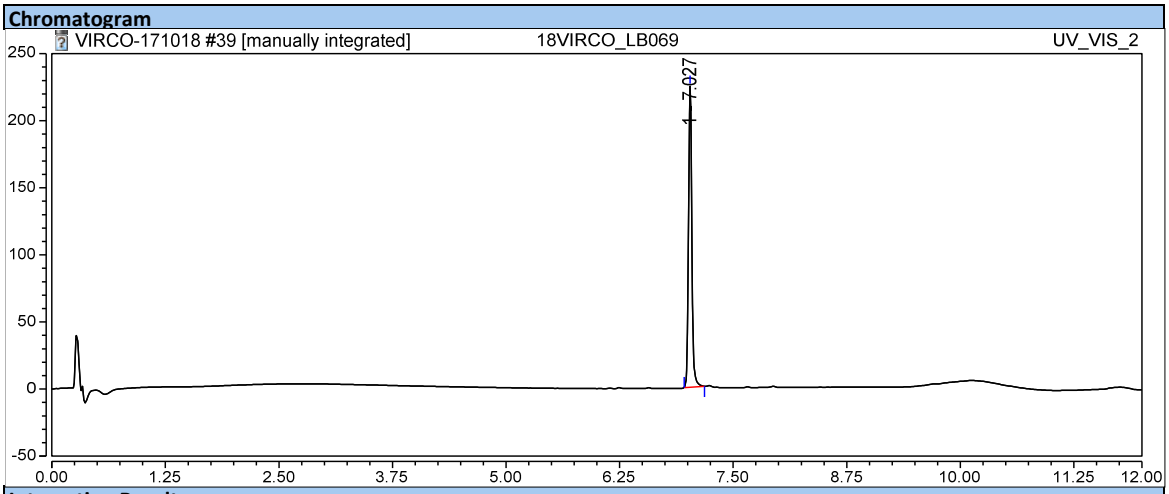
Figure S23: ^{1}H NMR (top) and ^{19}F spectra (down) of 5,10,15-tris(3',4',5'-trifluorophenyl)corrole **8** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

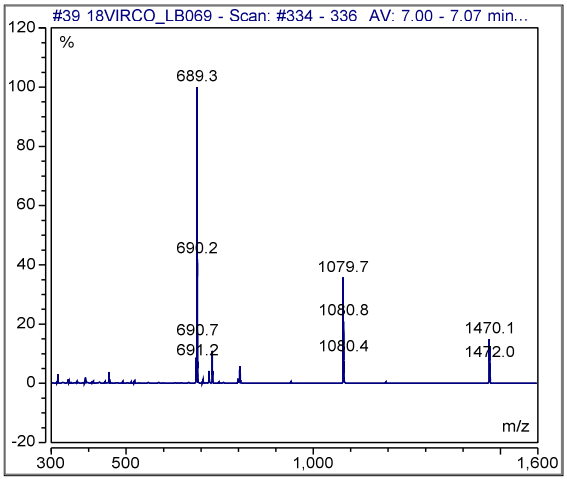
Injection Name:	**18VIRCO_LB069**	*Run Time (min):*	**12.00**
Vial Number:	**GB5**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**28/Feb/19 17:49**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.027	9.512	224.332	100.00	100.00	n.a.
Total:			**9.512**	**224.332**	**100.00**	**100.00**	



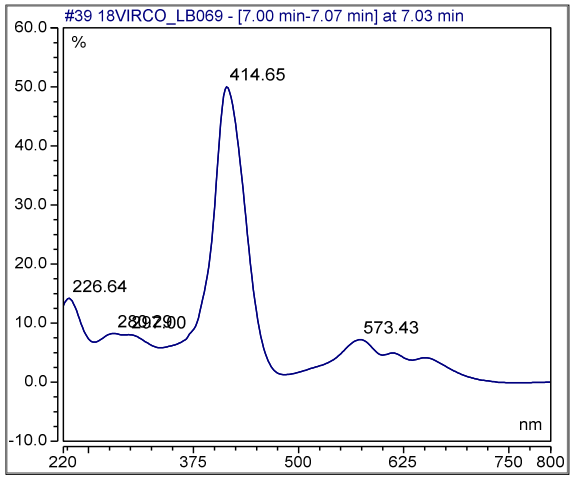
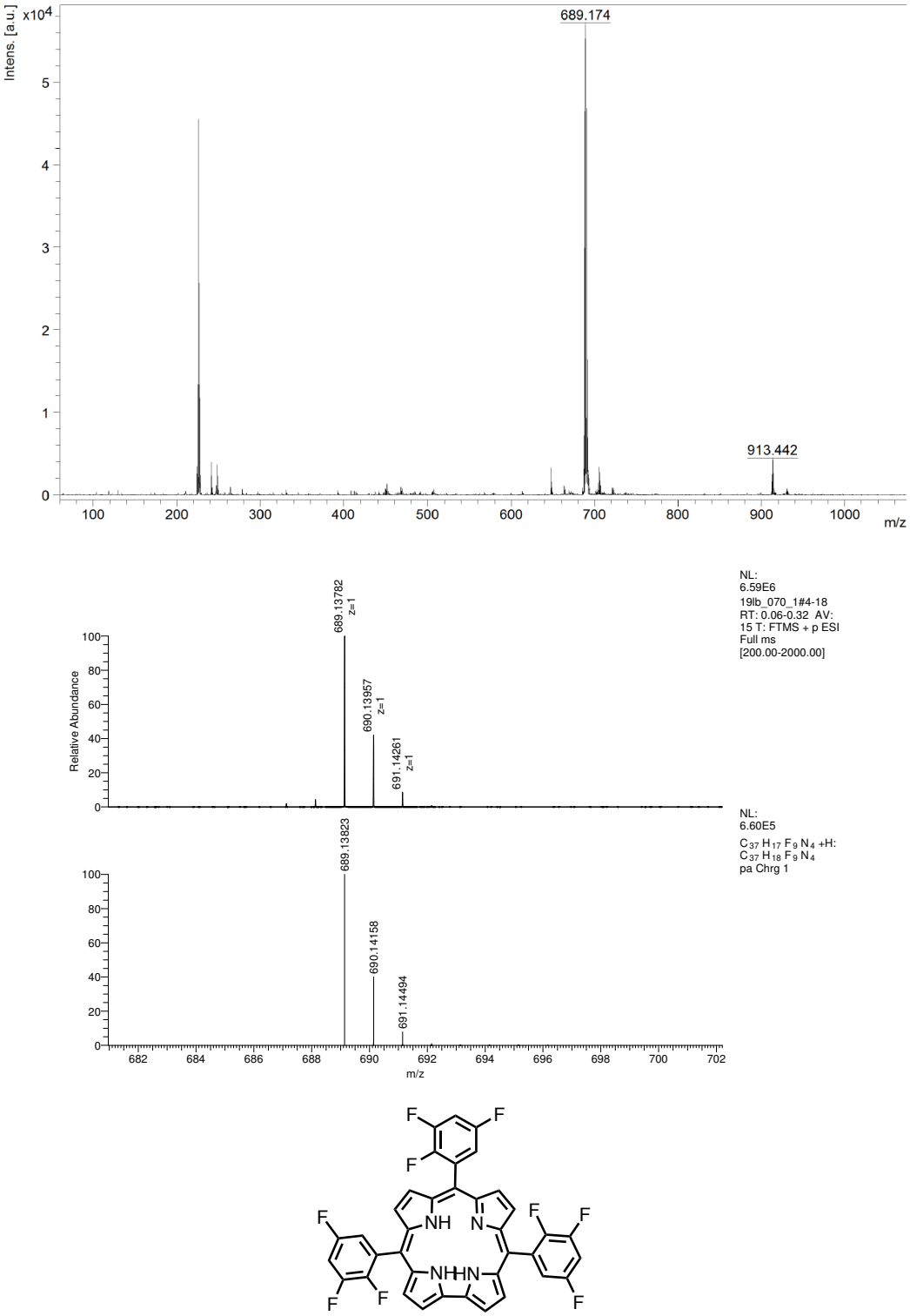


Figure S24: HPLC chromatogram of of 5,10,15-tris(3',4',5'-trifluorophenyl)corrole **8**.



Chemical Formula: $C_{37}H_{17}F_9N_4$
Exact Mass: 688.1310
Molecular Weight: 688.5566

Figure S25: MALDI/TOF LRMS and ESI HMRS mass spectrum of 5,10,15-tris(2',3',5'-trifluorophenyl)corrole **9**.

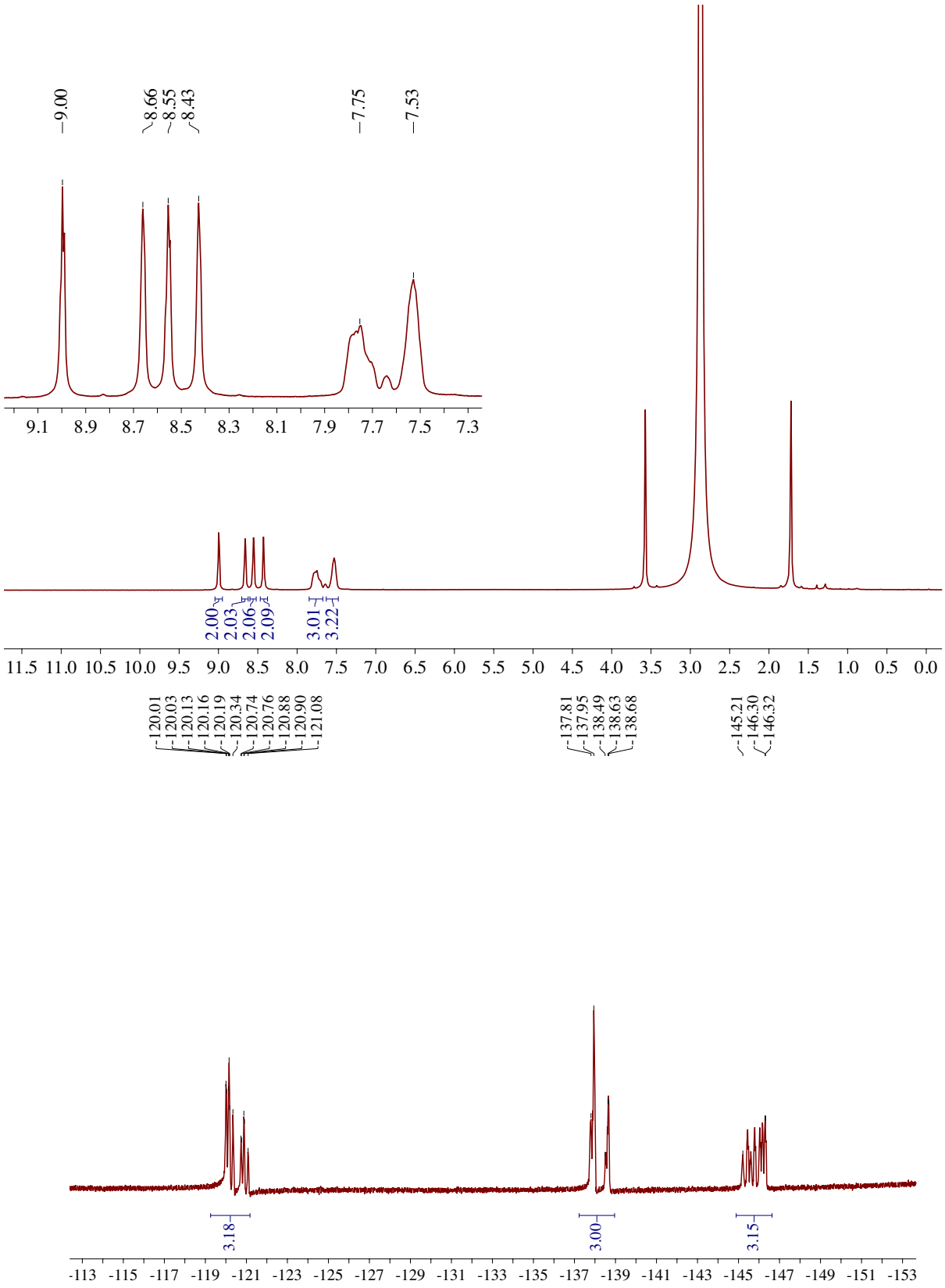


Figure S26: [1]H NMR (top) and [19]F spectra (down) of 5,10,15-tris(2',3',5'-trifluorophenyl)corrole **9** in THF-d_8 + one drop of hydrazine hydrate 64%.

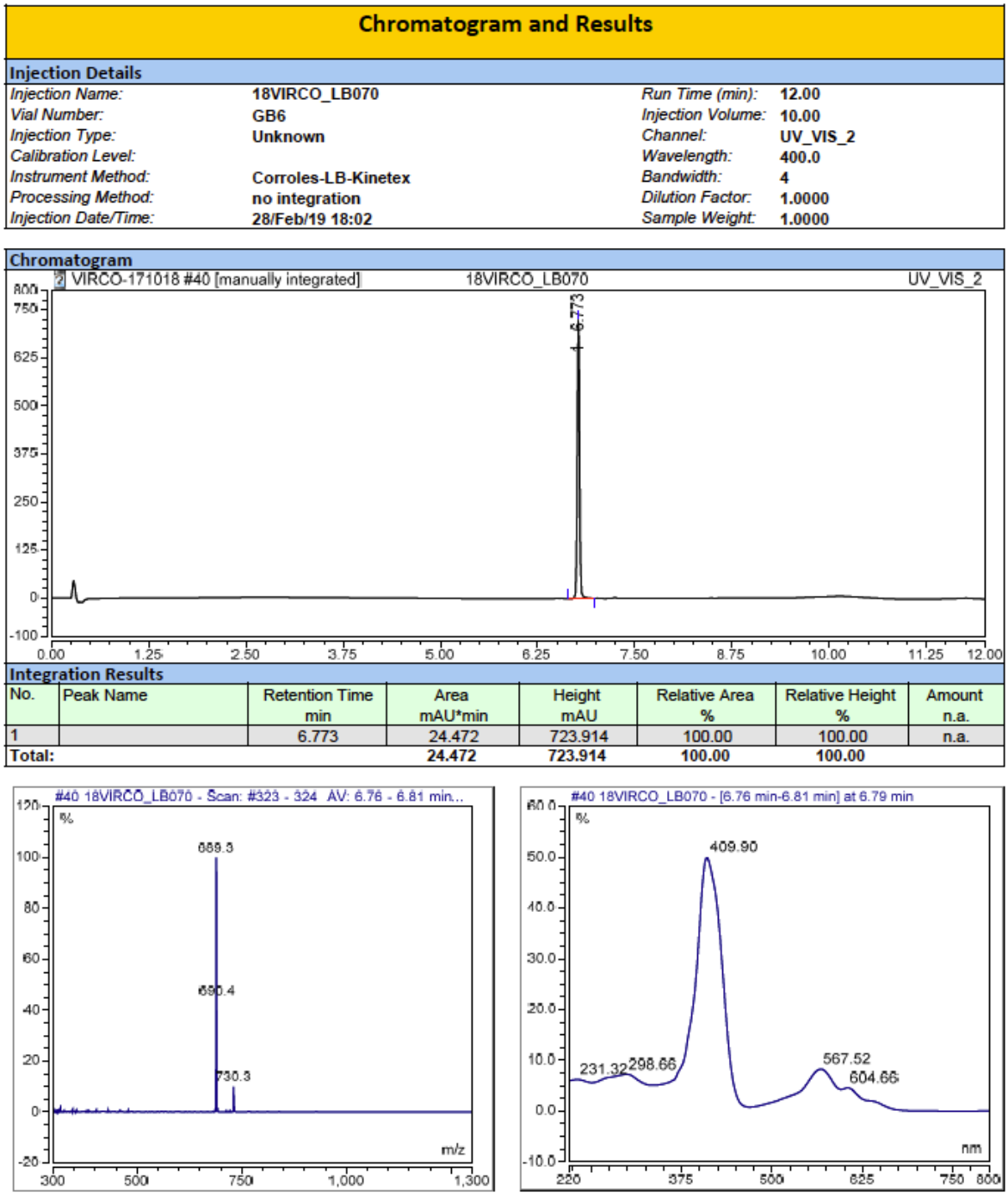
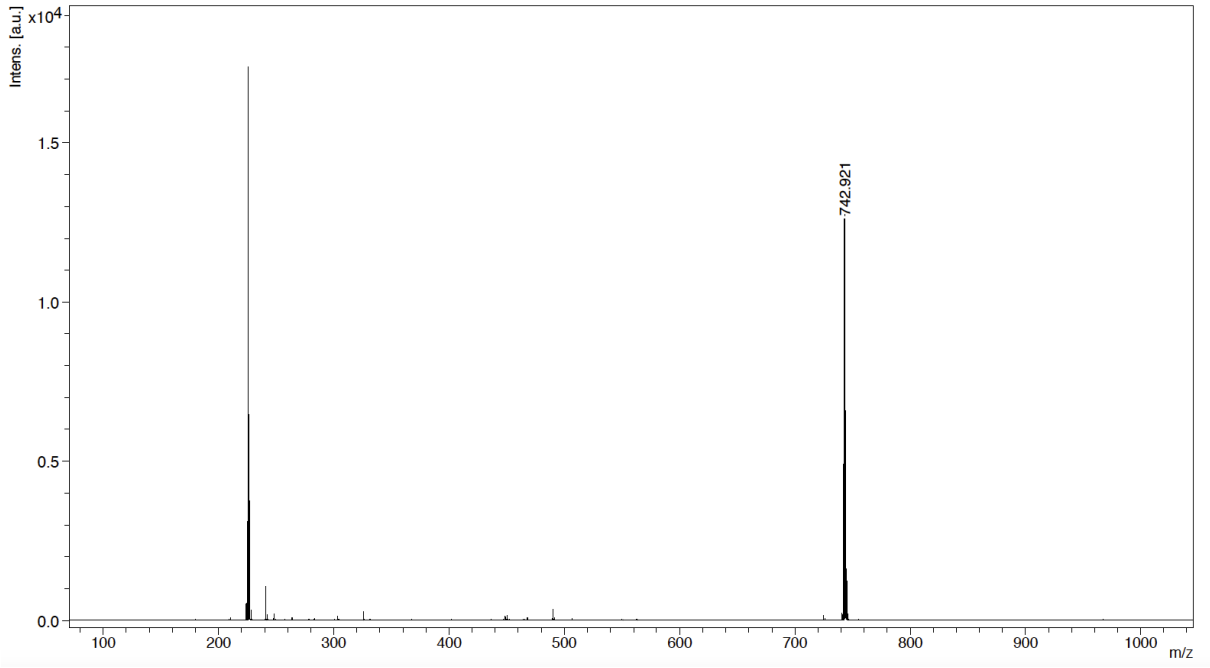
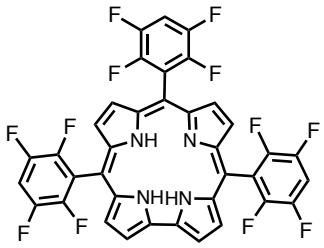


Figure S27: HPLC chromatogram of 5,10,15-tris(2',3',5'-trifluorophenyl)corrole **9**.





Chemical Formula: $C_{37}H_{14}F_{12}N_4$
Exact Mass: 742.1027
Molecular Weight: 742.5278

Figure S28: MALDI/TOF LRMS mass spectrum of 5,10,15-tris(2',3',5',6'-tetrafluorophenyl)corrole **10**.

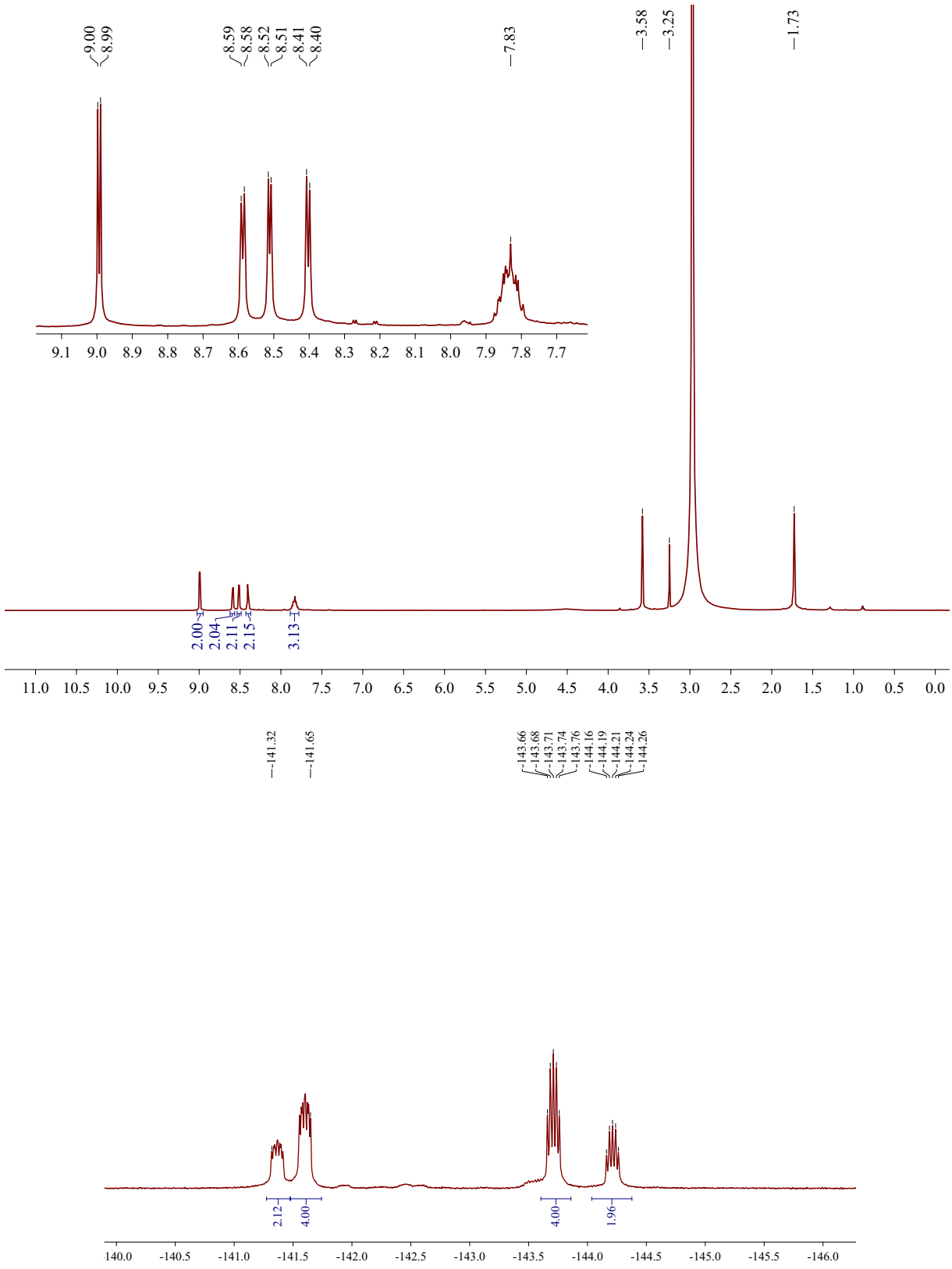


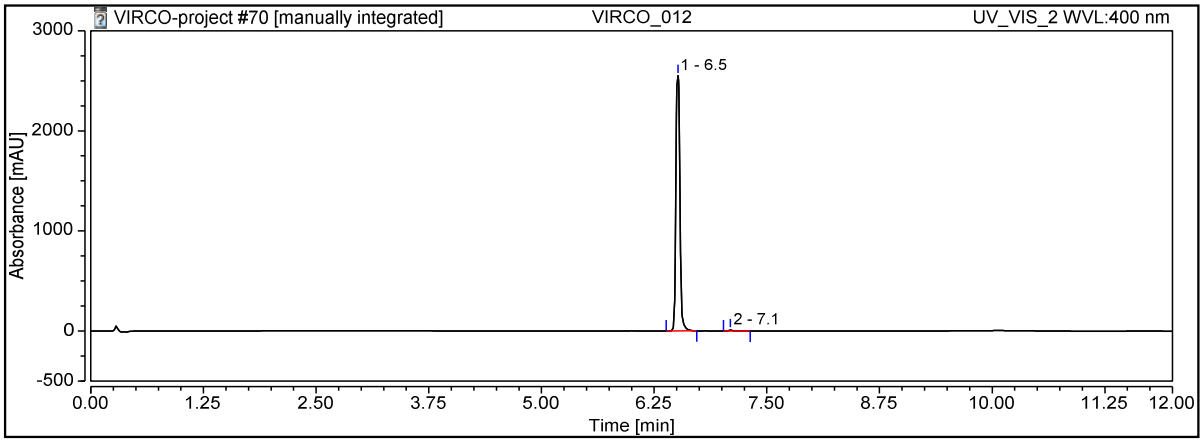
Figure S29: ^{1}H NMR (top) and ^{19}F spectra (down) of 5,10,15-tris(2',3',5',6'-tetrafluorophenyl)corrole **10** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

Injection Name:	**VIRCO_012**	*Run Time (min):*	**12.00**
Vial Number:	**BC6**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**06/Sep/18 10:38**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.513	135.073	2551.966	99.80	99.58	n.a.
2		7.097	0.266	10.848	0.20	0.42	n.a.
Total:			**135.339**	**2562.814**	**100.00**	**100.00**	

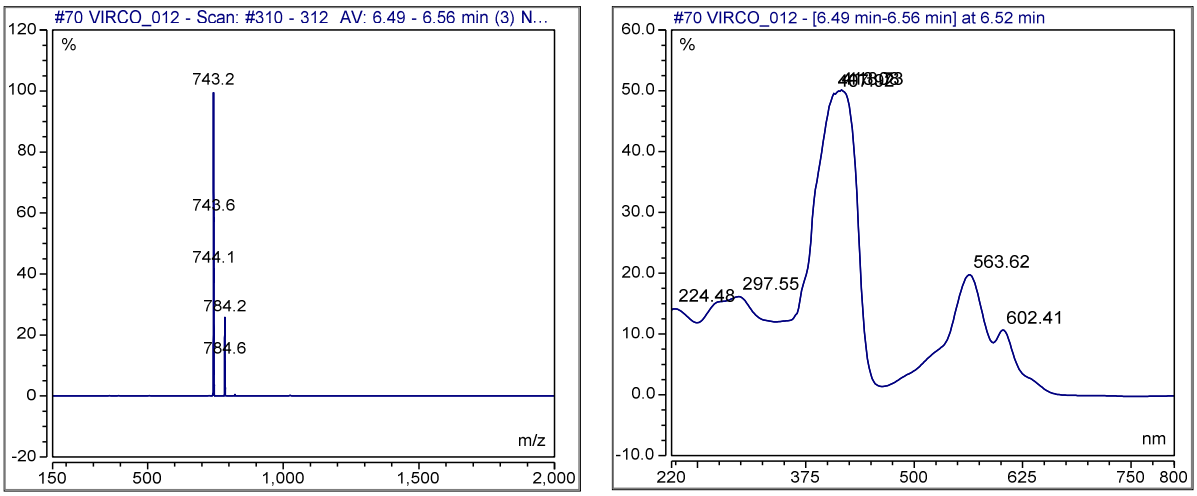
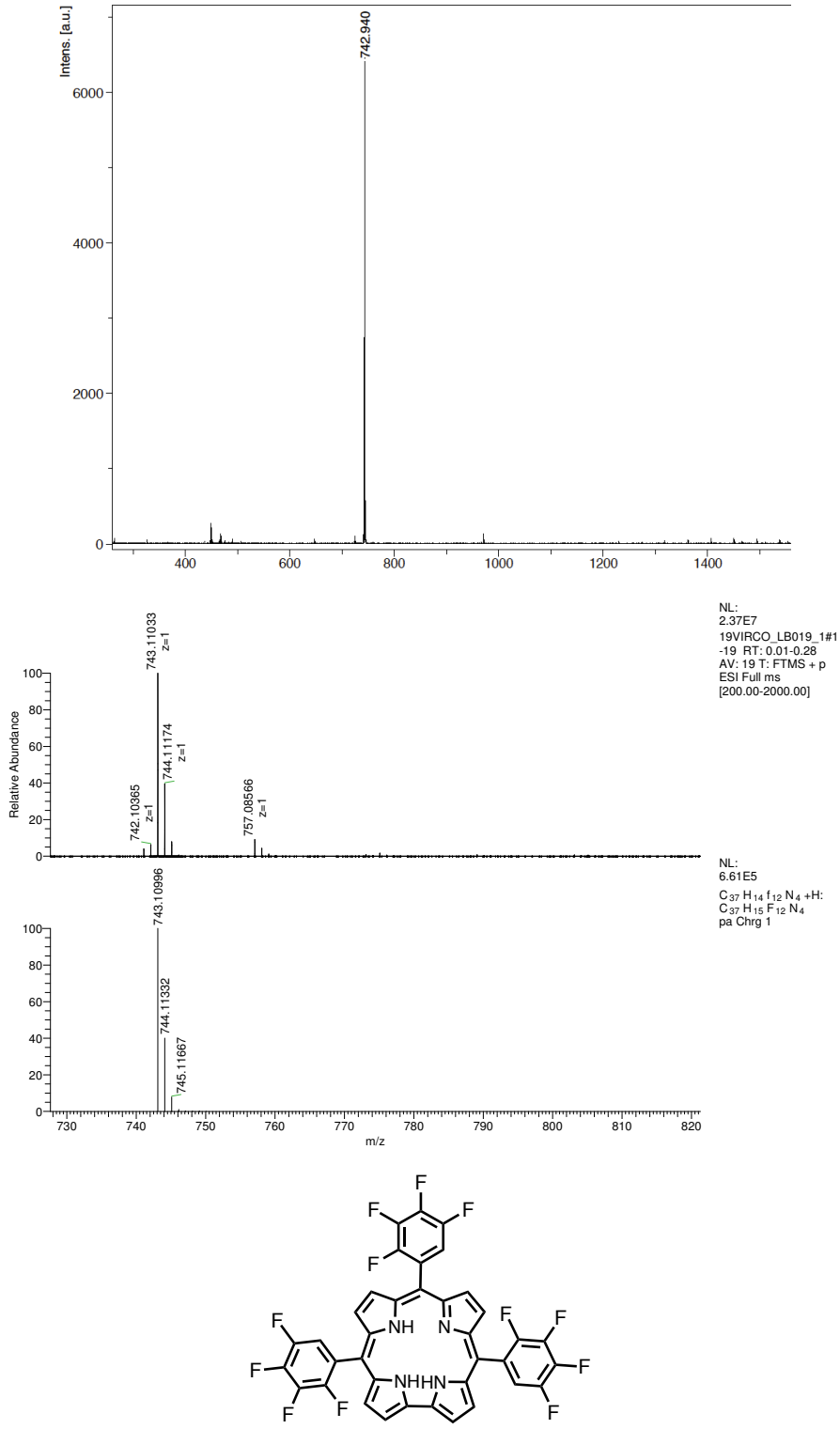


Figure S30: HPLC chromatogram of 5,10,15-tris(2',3',5',6'-tetrafluorophenyl)corrole **10**.



Chemical Formula: $C_{37}H_{14}F_{12}N_4$
Exact Mass: 742.1027
Molecular Weight: 742.5278

Figure S31: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,10,15-tris(2',3',4',5'-tetrafluorophenyl)corrole **11**.

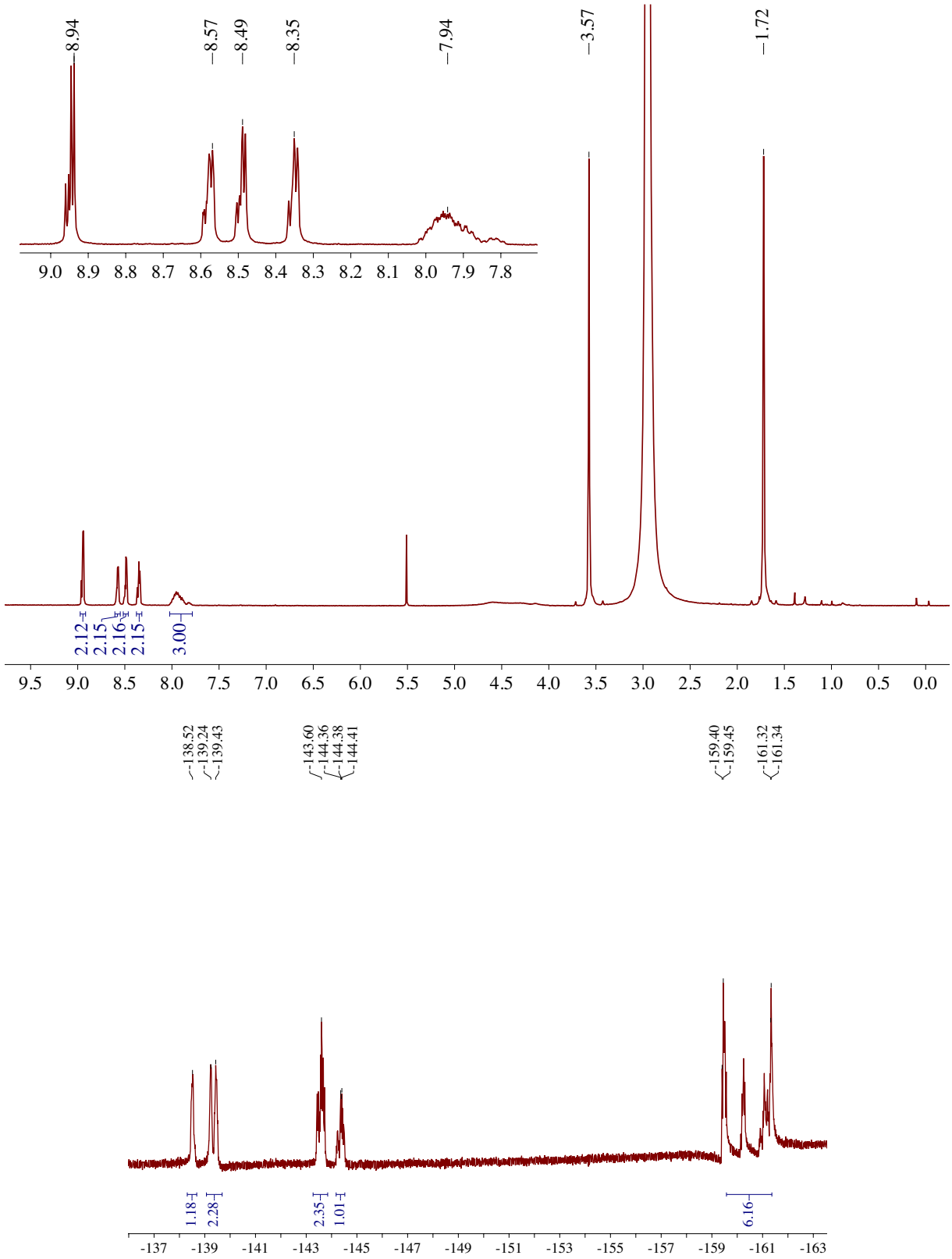


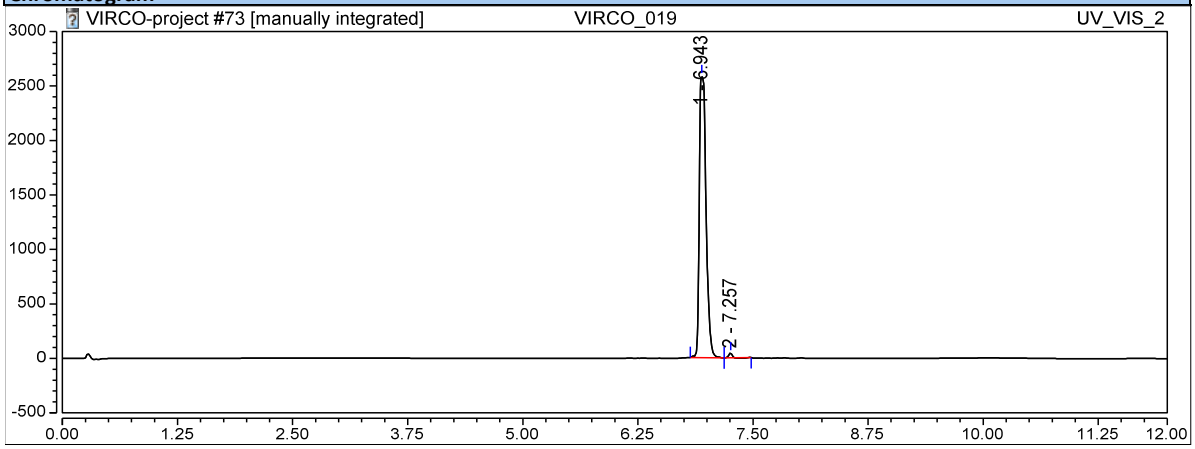
Figure S32: ^{1}H NMR (top) and ^{19}F spectra (down) of 5,10,15-tris(2',3',4',5'-tetrafluorophenyl)corrole **11** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

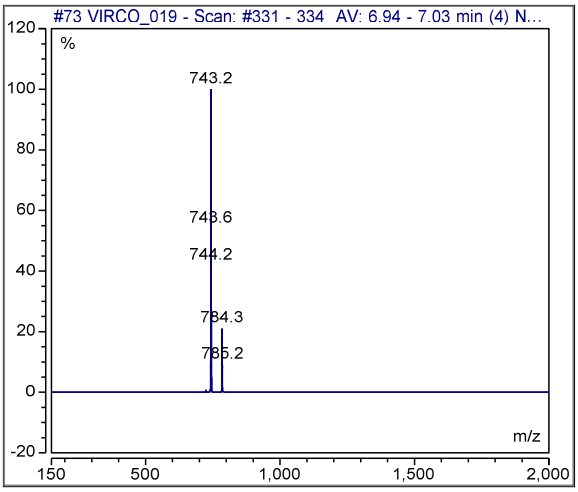
Injection Name:	**VIRCO_019**	*Run Time (min):*	**12.00**
Vial Number:	**RC3**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**06/Sep/18 18:45**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.943	219.028	2587.398	99.38	98.29	n.a.
2		7.257	1.367	45.117	0.62	1.71	n.a.
Total:			**220.395**	**2632.516**	**100.00**	**100.00**	



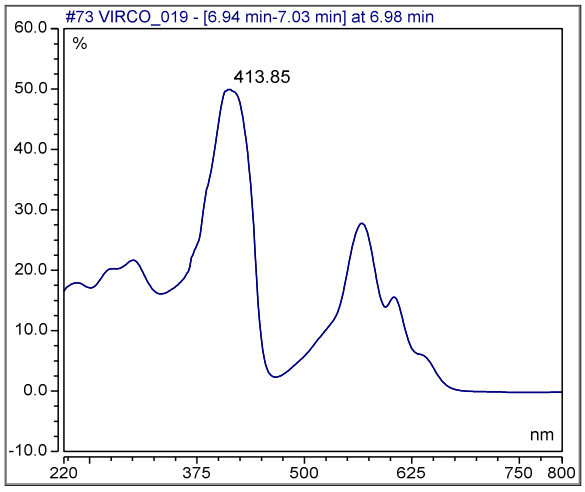
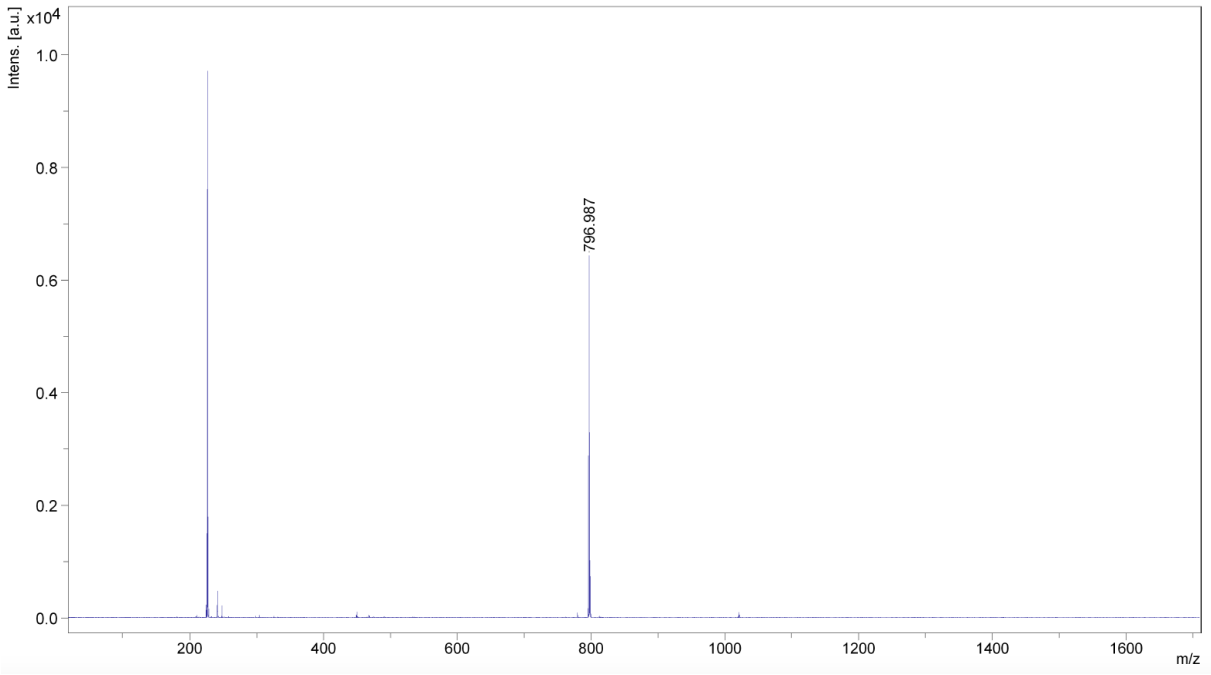
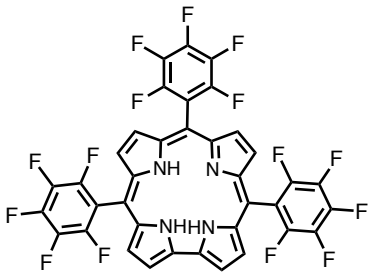


Figure S33: HPLC chromatogram of 5,10,15-tris(2',3',4',5'-tetrafluorophenyl)corrole **11**.





Chemical Formula: $C_{37}H_{11}F_{15}N_4$
Exact Mass: 796.0744
Molecular Weight: 796.4990

Figure S34: MALDI/TOF LRMS mass spectrum of 5,10,15-tris(pentafluorophenyl)corrole **12**.

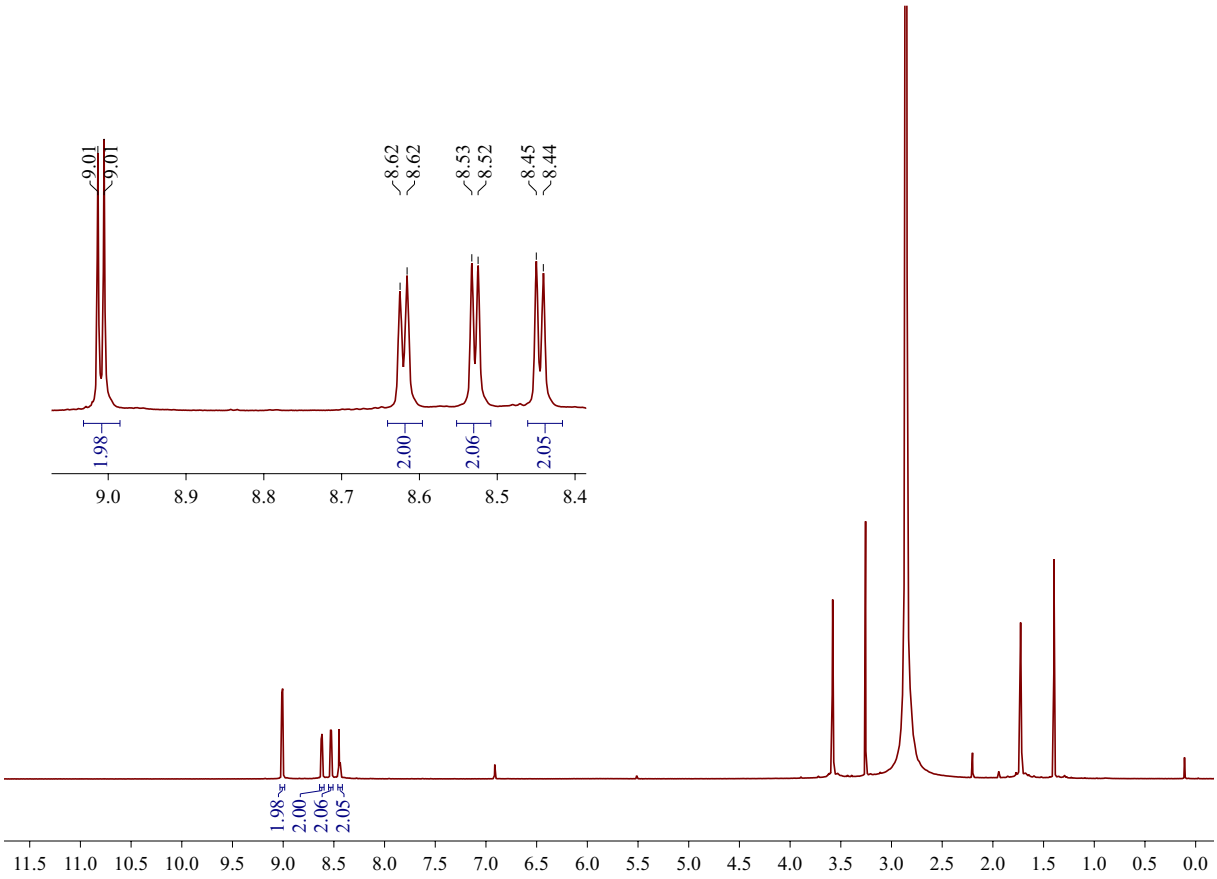


Figure S35: ^{1}H NMR spectrum of 5,10,15-tris(pentafluorophenyl)corrole **12** in THF-d_8 + one drop of hydrazine hydrate 64%.

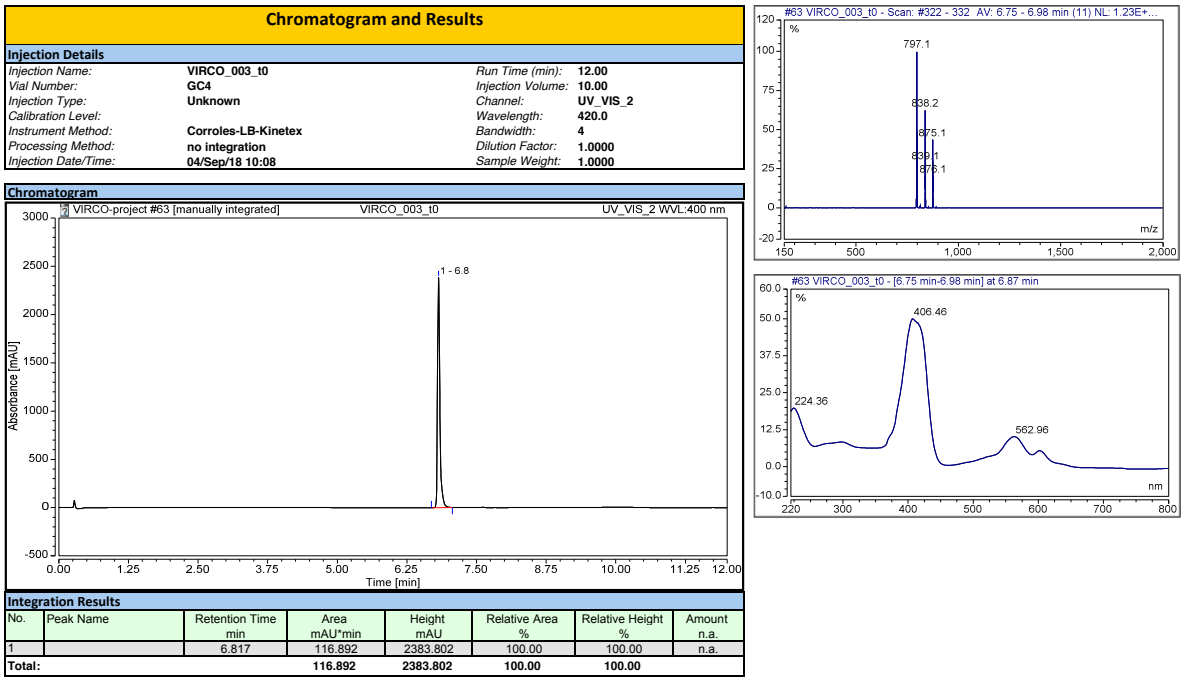
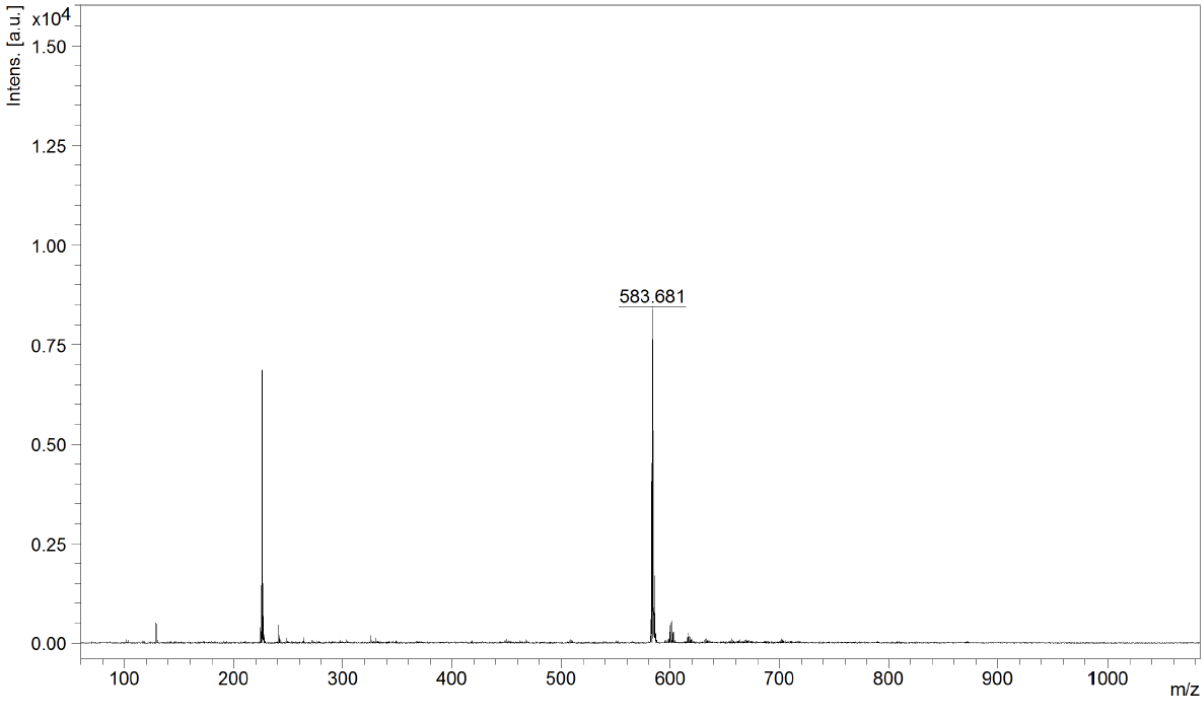
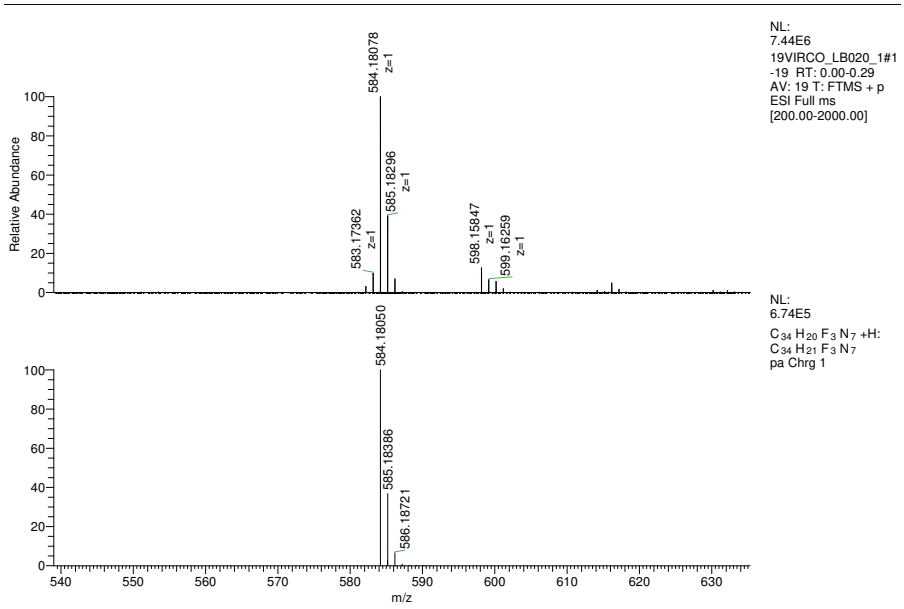
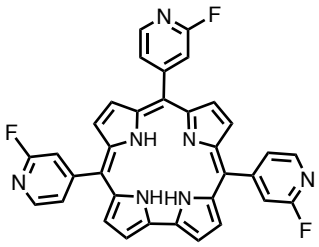


Figure S36: HPLC chromatogram of 5,10,15-tris(pentafluorophenyl)corrole **12**.







Chemical Formula: $C_{34}H_{20}F_3N_7$
Exact Mass: 583.1732
Molecular Weight: 583.5782

Figure S37: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,10,15-tris(2'-fluoropyrid-4'-yl)corrole **13**.

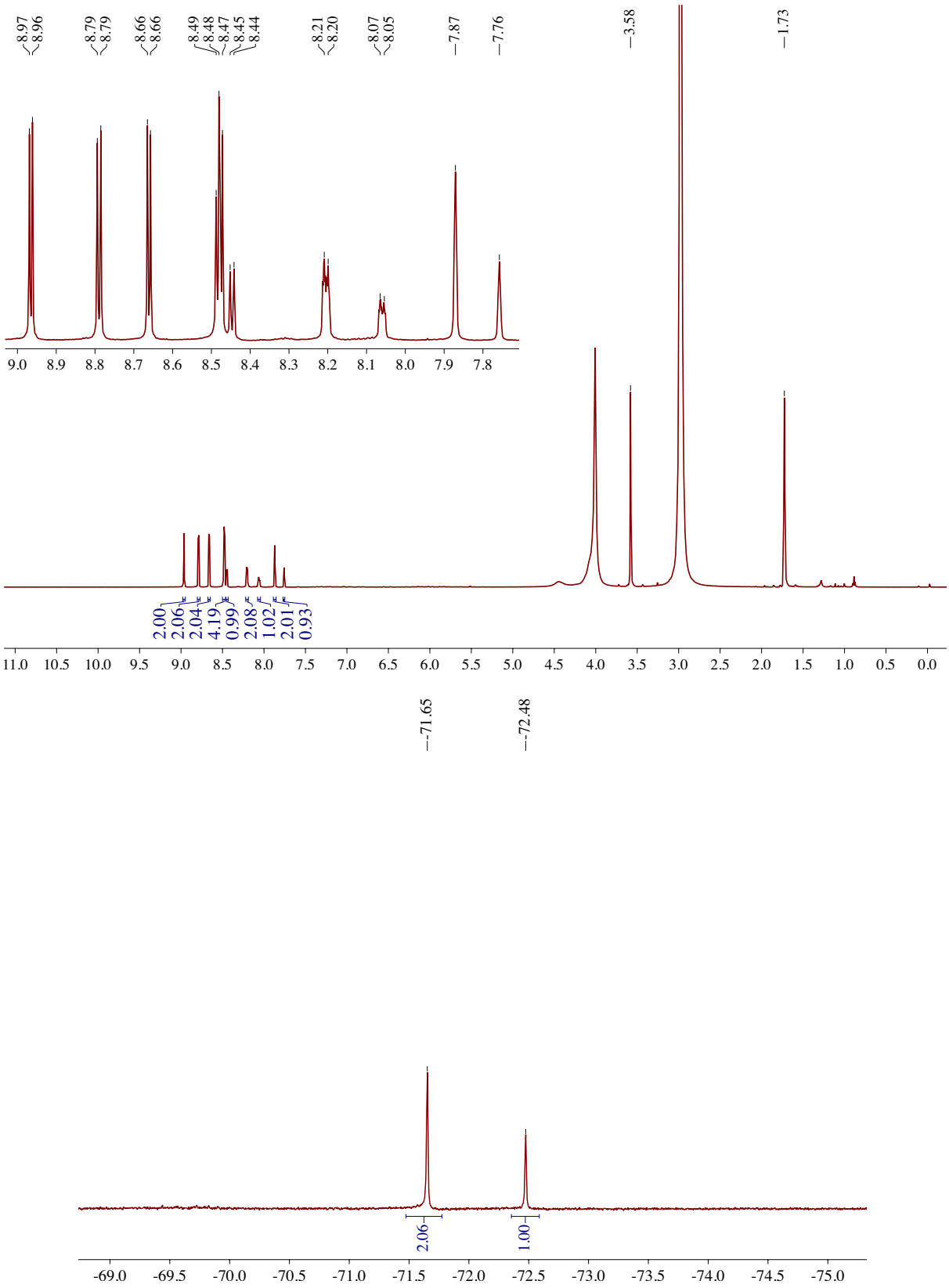


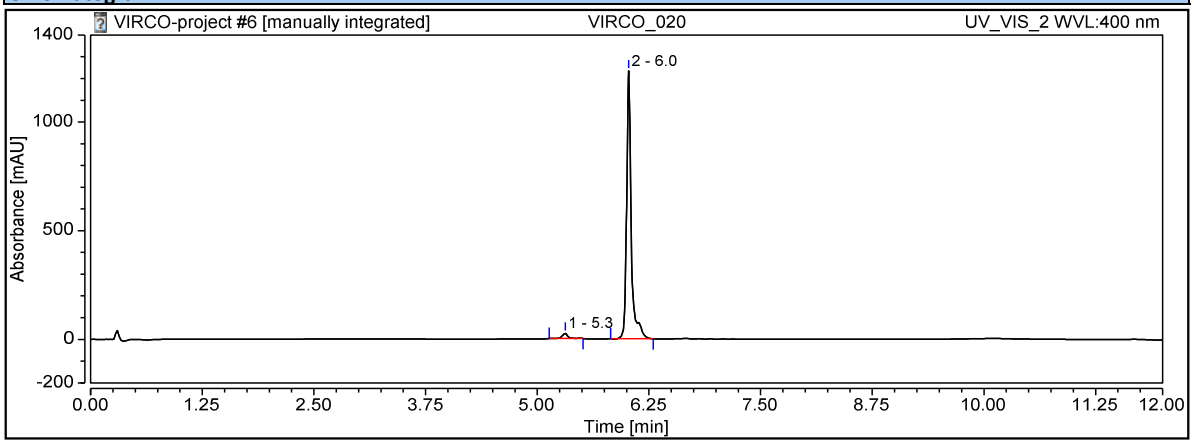
Figure S38: [1]H NMR spectrum of 5,10,15-tris(2'-fluoropyrid-4'-yl)corrole **13** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

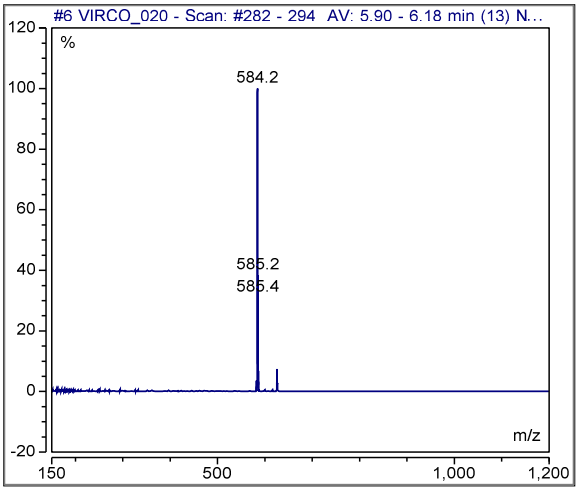
Injection Name:	**VIRCO_020**	*Run Time (min):*	**12.00**
Vial Number:	**RB5**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**02/May/18 16:09**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.313	1.792	24.478	2.38	1.95	n.a.
2		6.023	73.380	1232.367	97.62	98.05	n.a.
Total:			**75.172**	**1256.845**	**100.00**	**100.00**	



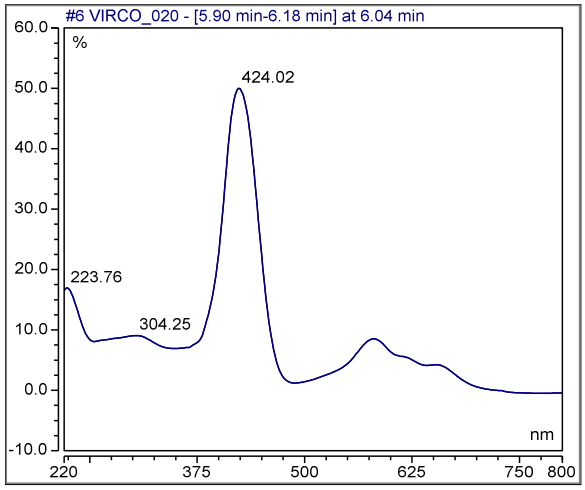
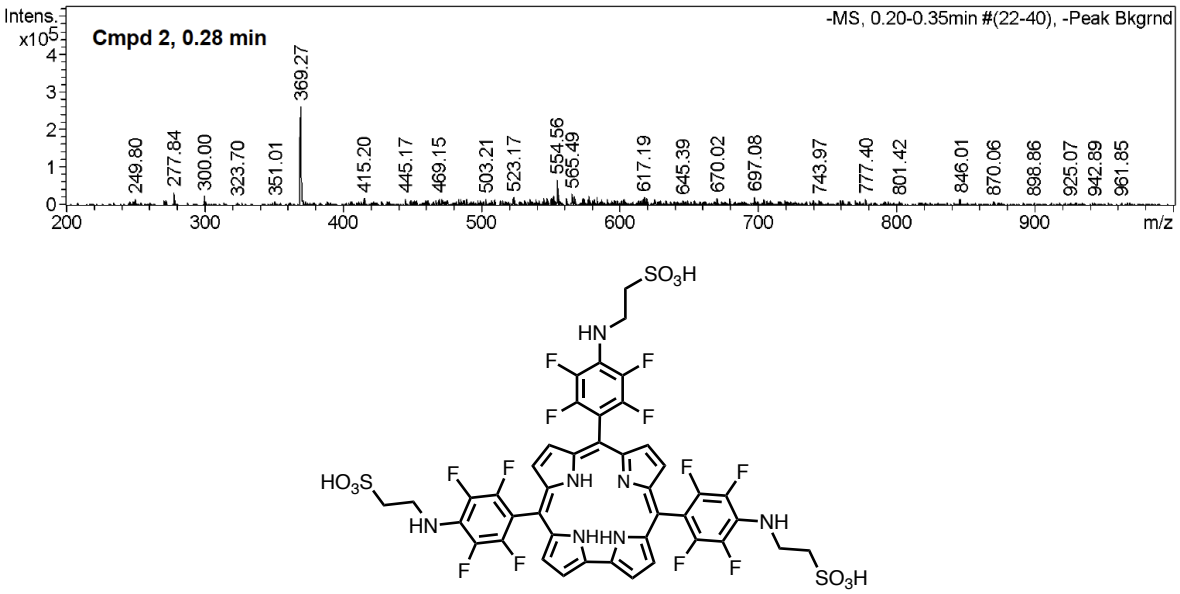


Figure S39: HPLC chromatogram of 5,10,15-tris(2'-fluoropyrid-4'-yl)corrole **13**.



Chemical Formula: $C_{43}H_{29}F_{12}N_7O_9S_3$

Exact Mass: 1111.0997

Exact Mass $[M-3H]^{3-}$: 369.36

Figure S40: ESI LRMS mass spectrum of 5,10,15-tris(4-((2-sulfoethyl)amino)-2,3,5,6-tetrafluorophenyl)corrole **14**.

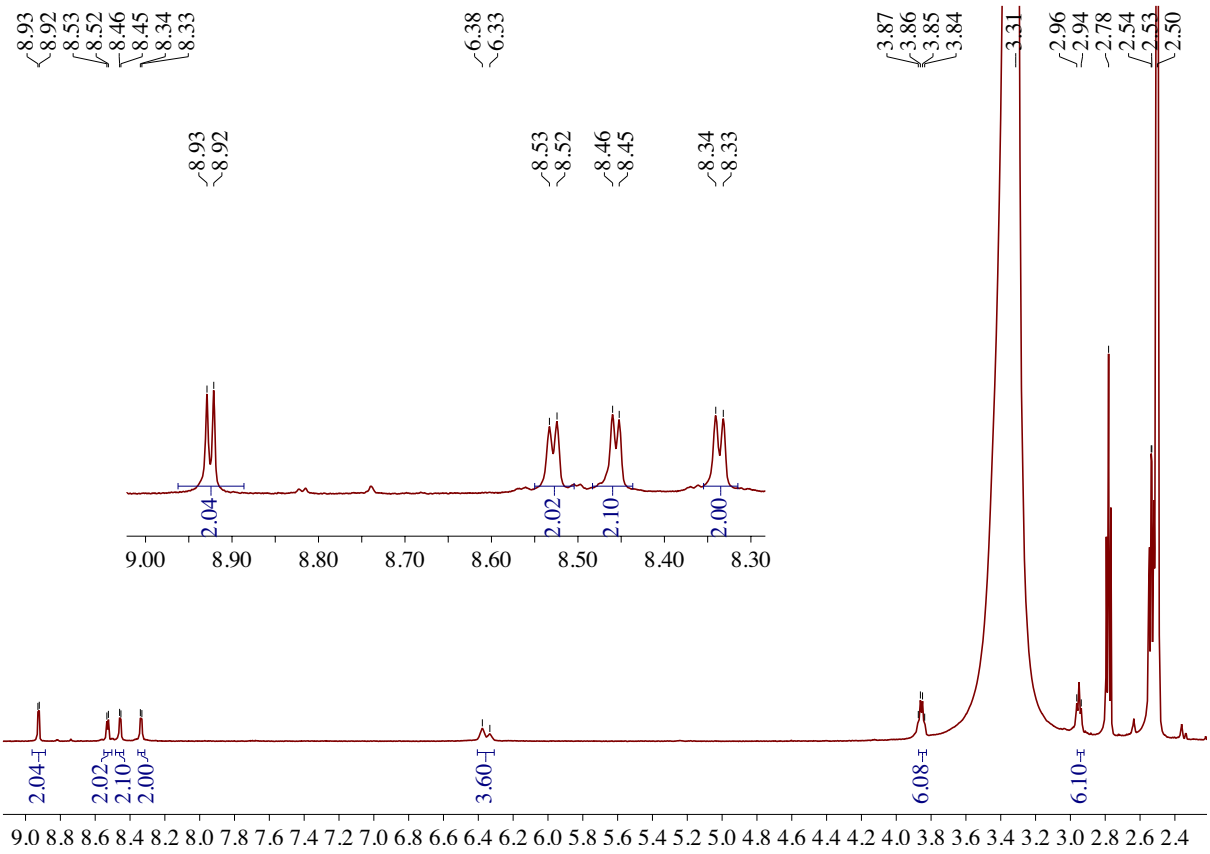
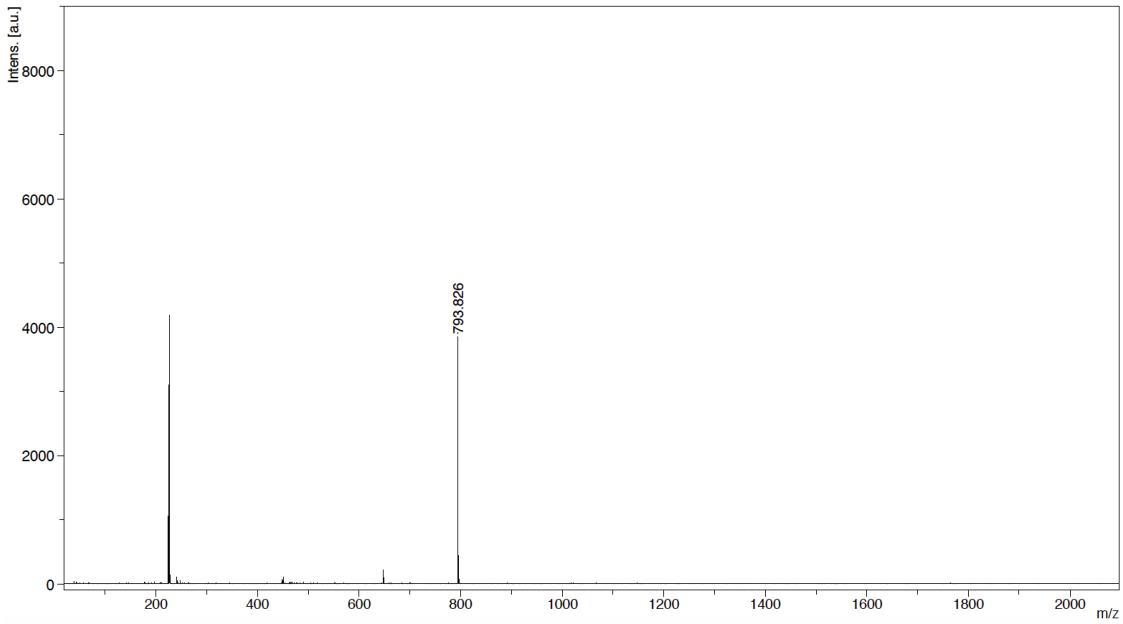
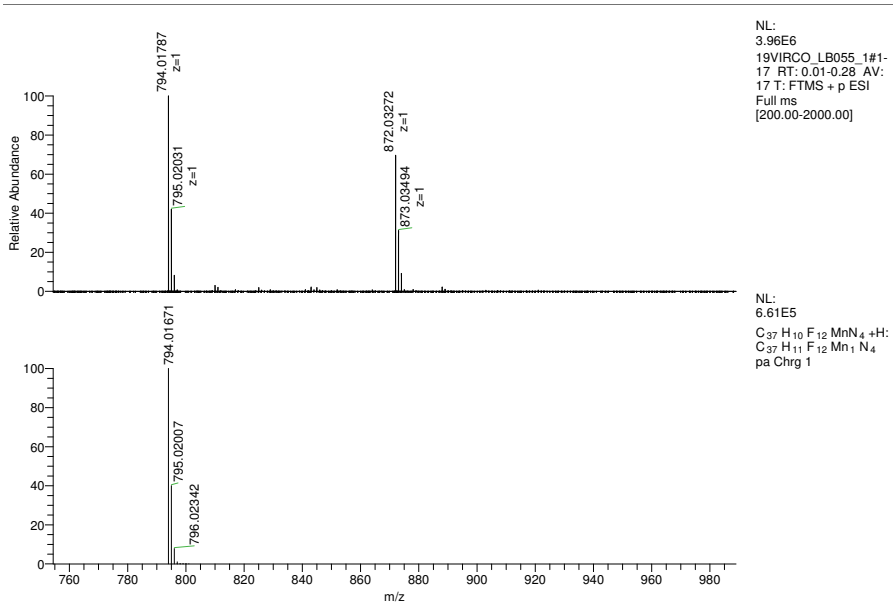
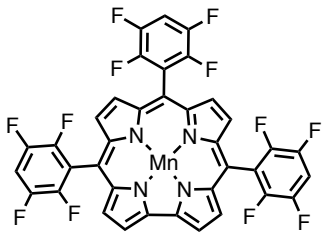


Figure S41: ^{1}H NMR spectrum of 5,10,15-tris(4-((2-sulfoethyl)amino)-2,3,5,6-tetrafluorophenyl)corrole **14** in DMSO-d_6 + one drop of hydrazine hydrate 64%.







Chemical Formula: $C_{37}H_{11}F_{12}MnN_4$
Exact Mass: 794.0173
Molecular Weight: 794.4419

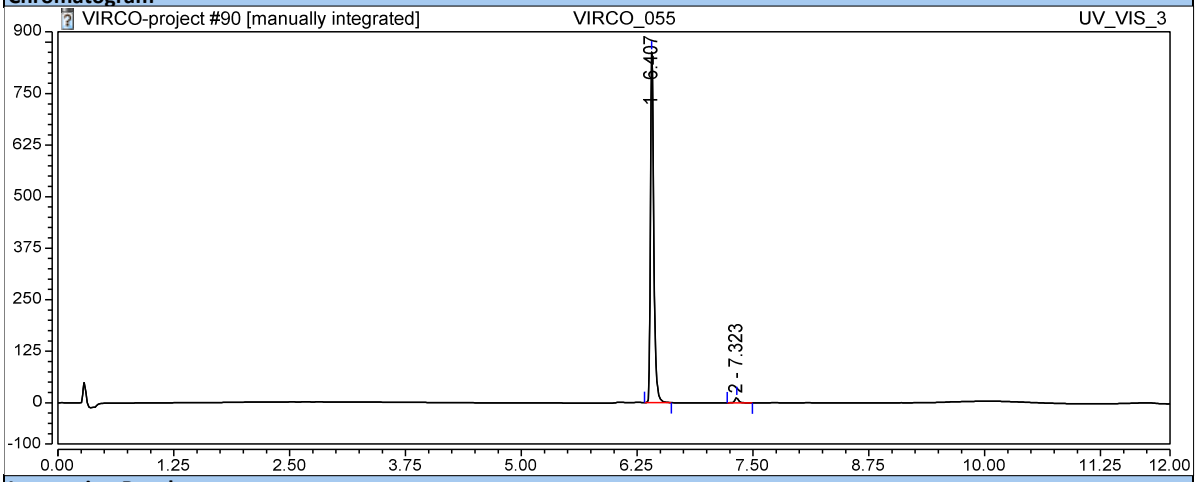
Figure S42: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,10,15-tris(2',3',5',6'-tetrafluorophenyl)corrole Mn(III) **15**.

Chromatogram and Results

Injection Details

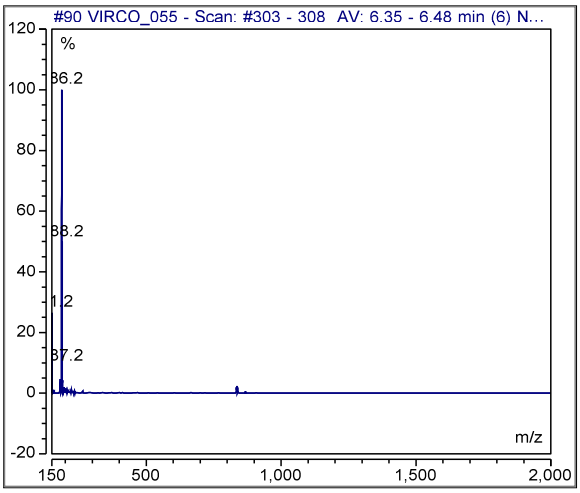
Injection Name:	**VIRCO_055**	*Run Time (min):*	**12.00**
Vial Number:	**GD6**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_3**
Calibration Level:		*Wavelength:*	**440.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**25/Sep/18 10:04**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.407	35.752	850.894	98.43	98.55	n.a.
2		7.323	0.570	12.532	1.57	1.45	n.a.
Total:			**36.321**	**863.426**	**100.00**	**100.00**	



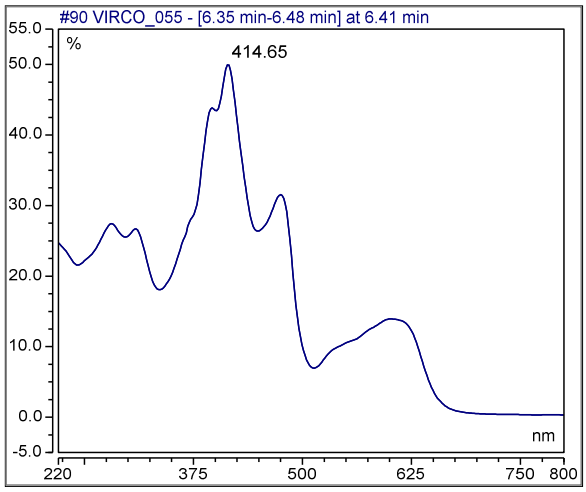
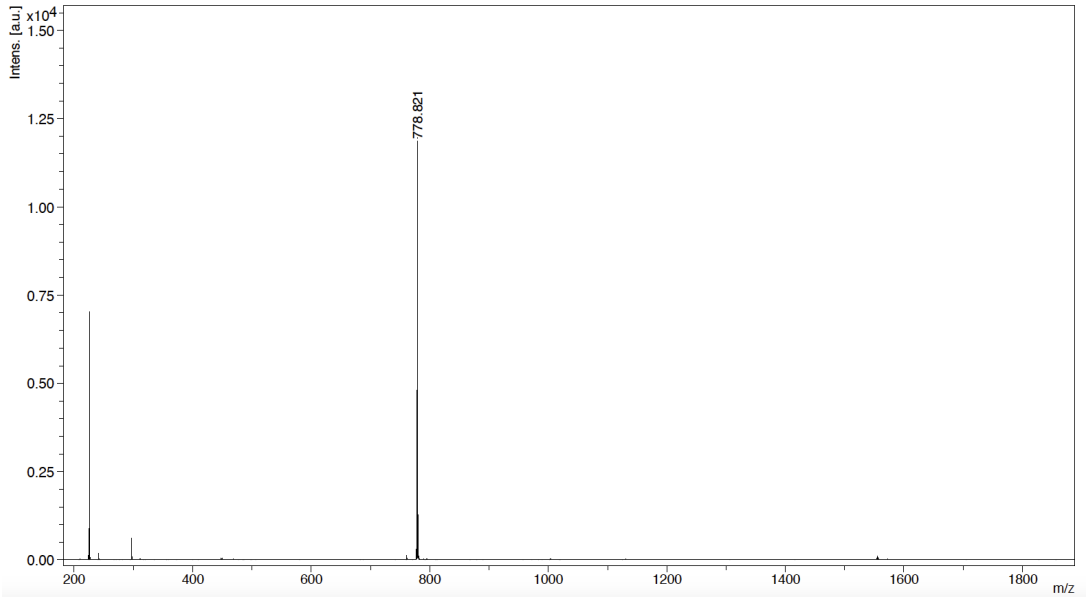
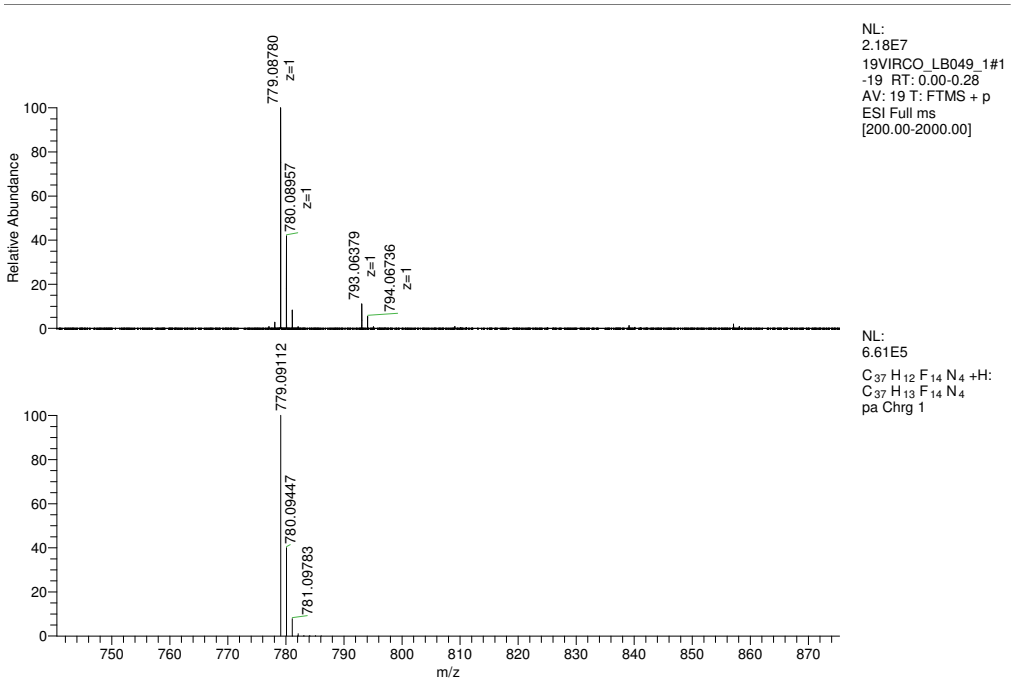
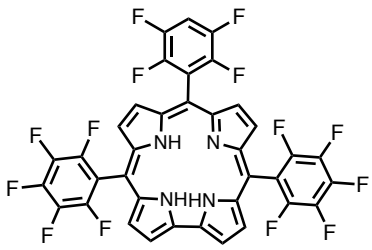


Figure S43: HPLC chromatogram of 5,10,15-tris(2',3',5',6'-tetrafluorophenyl)-corrole Mn(III) **15**.







Chemical Formula: $C_{37}H_{12}F_{14}N_4$
Exact Mass: 778.0838
Molecular Weight: 778.5086

Figure S44: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(pentafluorophenyl)-10-(2',3',5',6'-tetrafluorophenyl)corrole **16**.

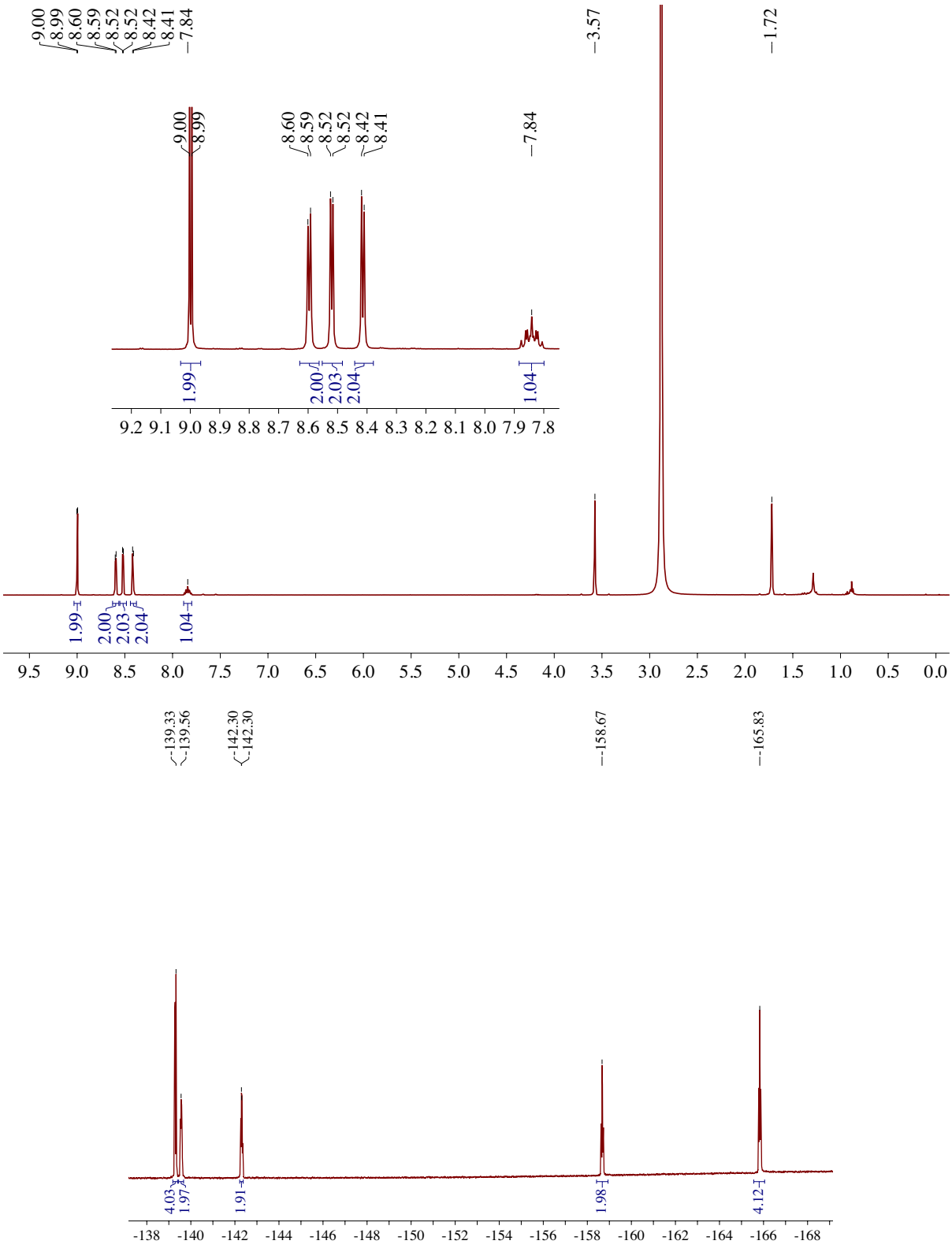


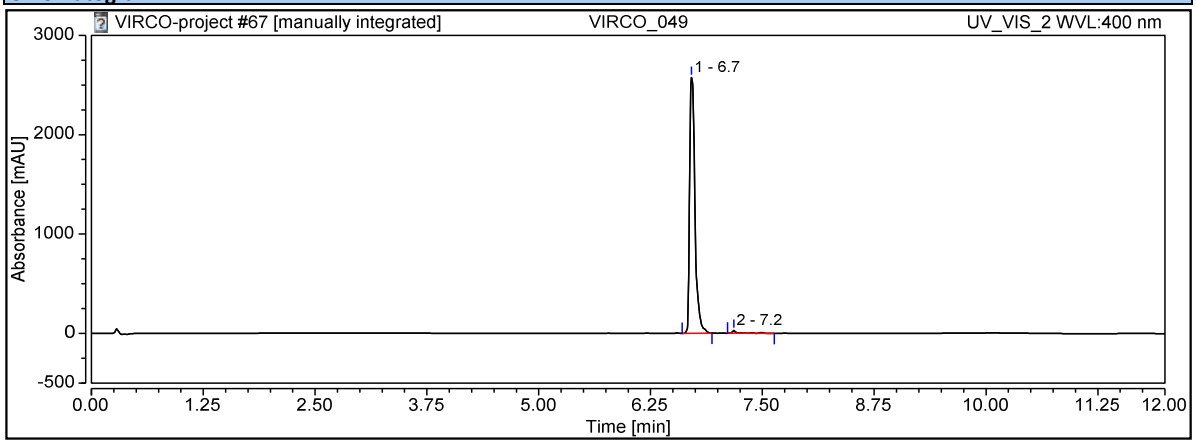
Figure S45: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(pentafluorophenyl)-15-(2',3',5',6'-tetrafluorophenyl)corrole **16** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

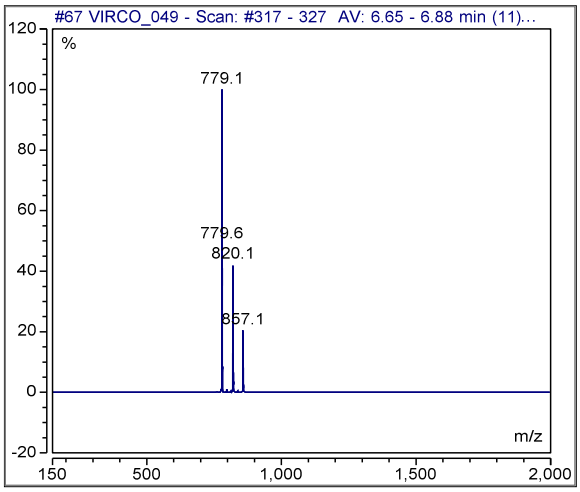
Injection Name:	**VIRCO_049**	*Run Time (min):*	**12.00**
Vial Number:	**RD5**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**420.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**04/Sep/18 19:04**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.707	179.863	2574.234	98.99	98.85	n.a.
2		7.180	1.835	30.021	1.01	1.15	n.a.
Total:			**181.697**	**2604.255**	**100.00**	**100.00**	



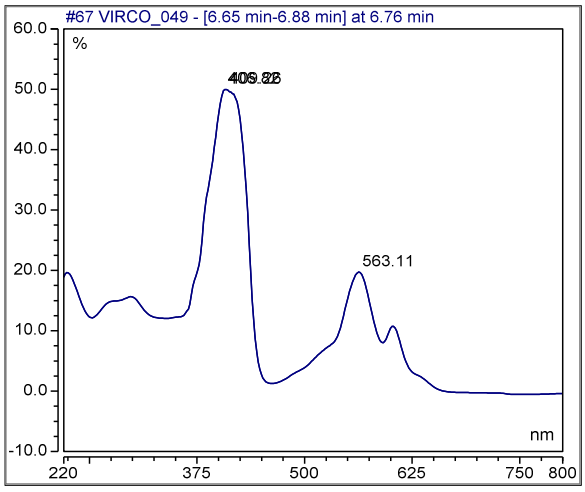
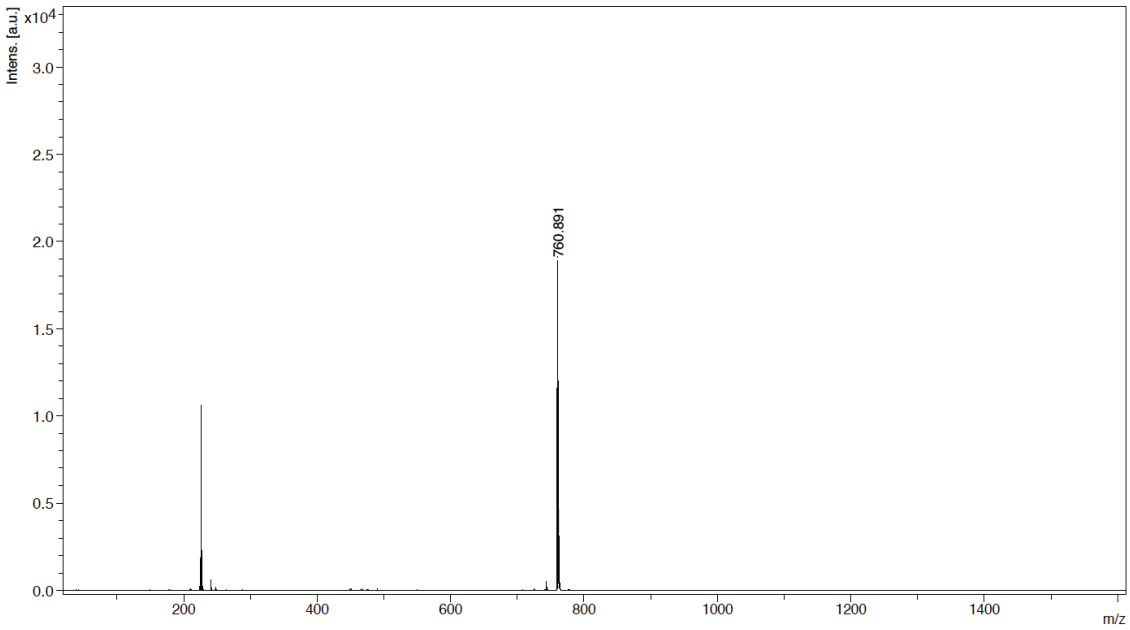
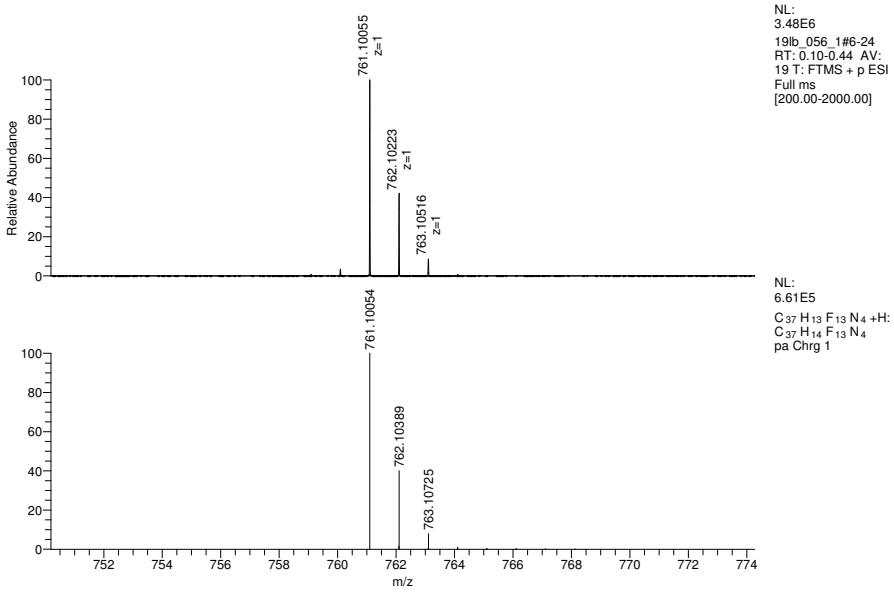
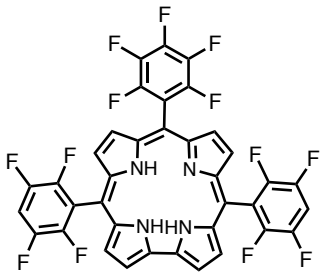


Figure S46: HPLC chromatogram of 5,15-bis(pentafluorophenyl)-10-(2',3',5',6'-tetrafluorophenyl)corrole **16**.







Chemical Formula: $C_{37}H_{13}F_{13}N_4$
Exact Mass: 760.0933
Molecular Weight: 760.5182

Figure S47: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pentafluorophenyl)corrole **17**.

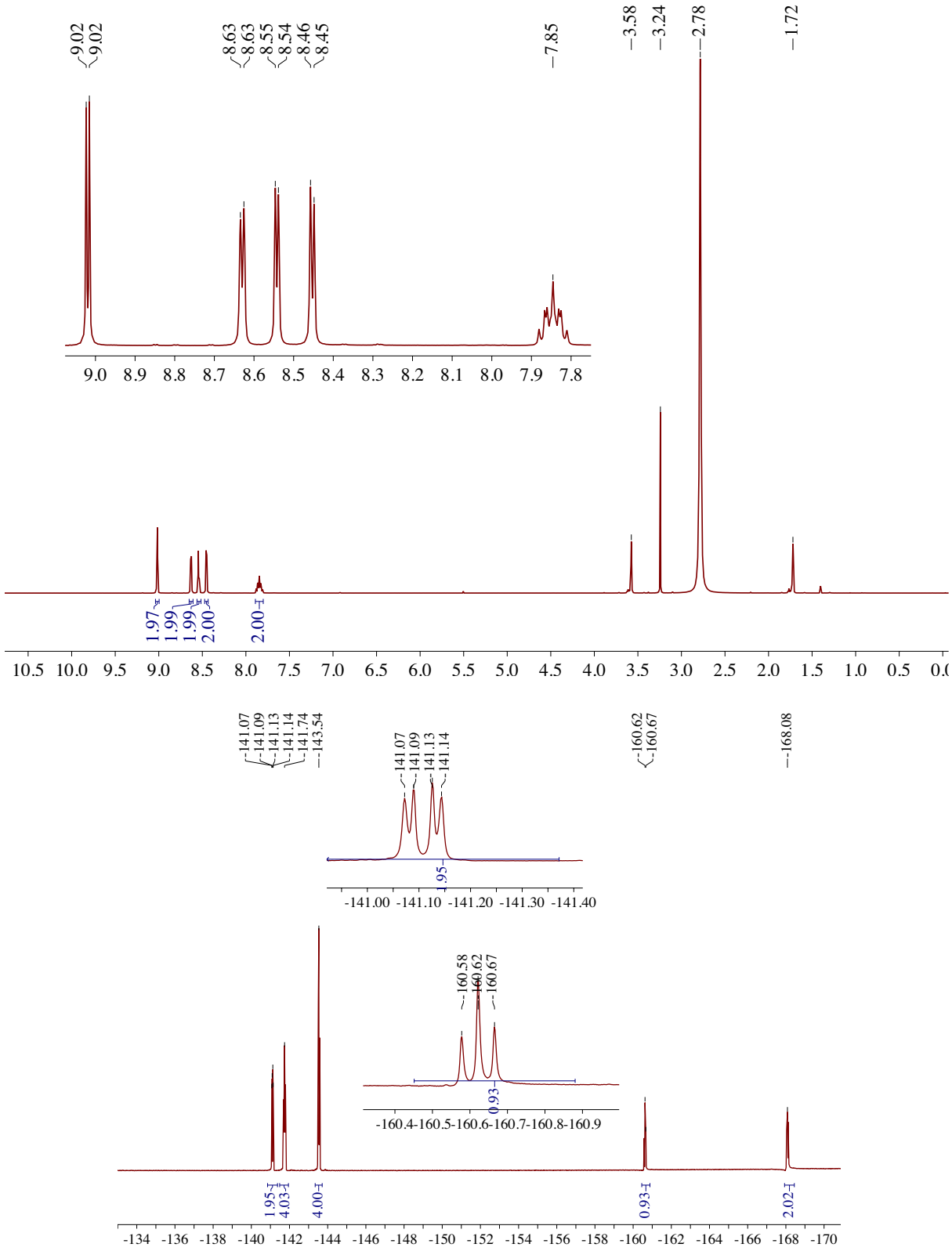


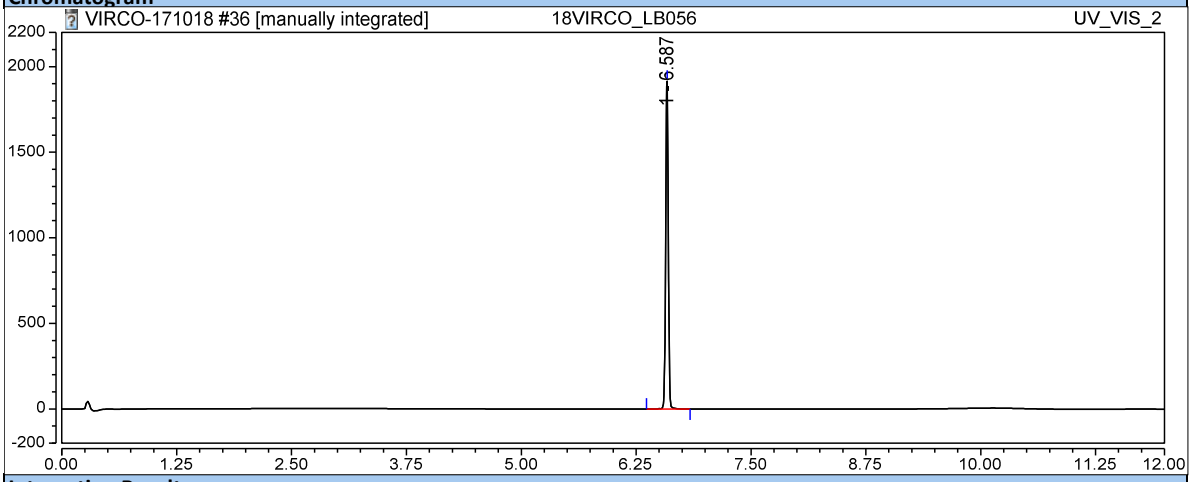
Figure S48: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pentafluorophenyl)corrole **17** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

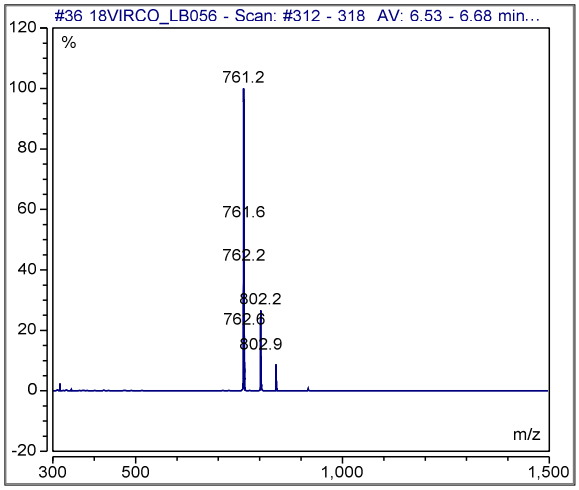
Injection Name:	**18VIRCO_LB056**	*Run Time (min):*	**12.00**
Vial Number:	**BA5**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**28/Feb/19 16:00**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.587	62.445	1915.493	100.00	100.00	n.a.
Total:			**62.445**	**1915.493**	**100.00**	**100.00**	



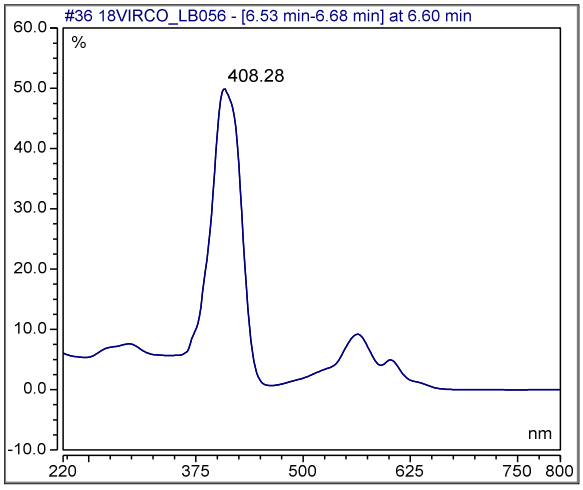
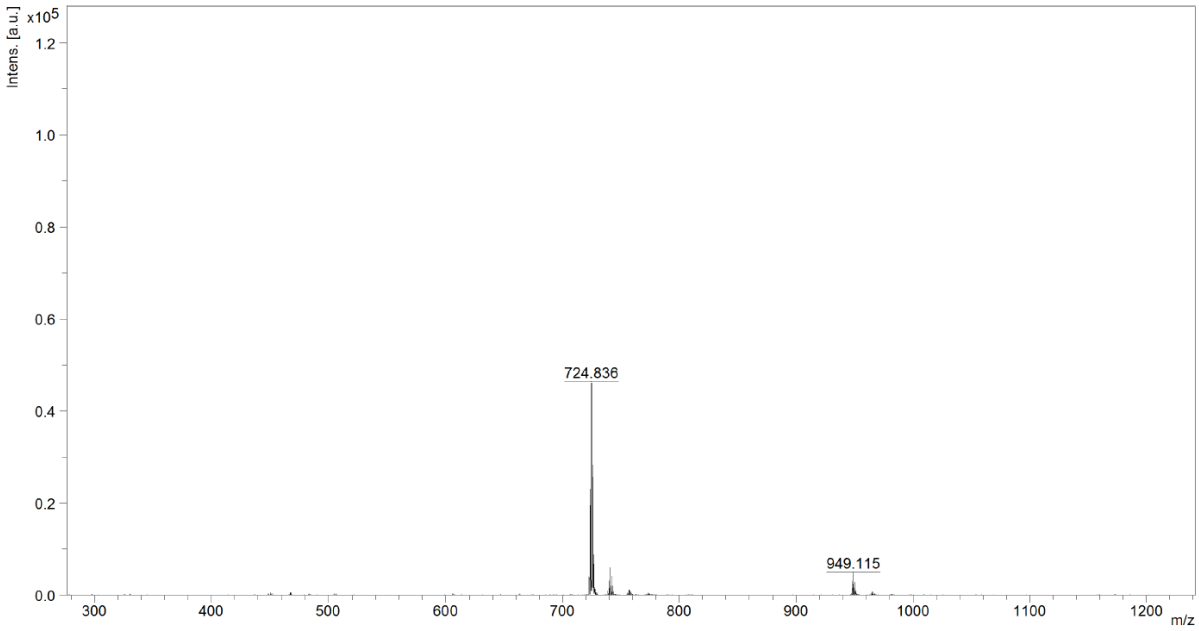
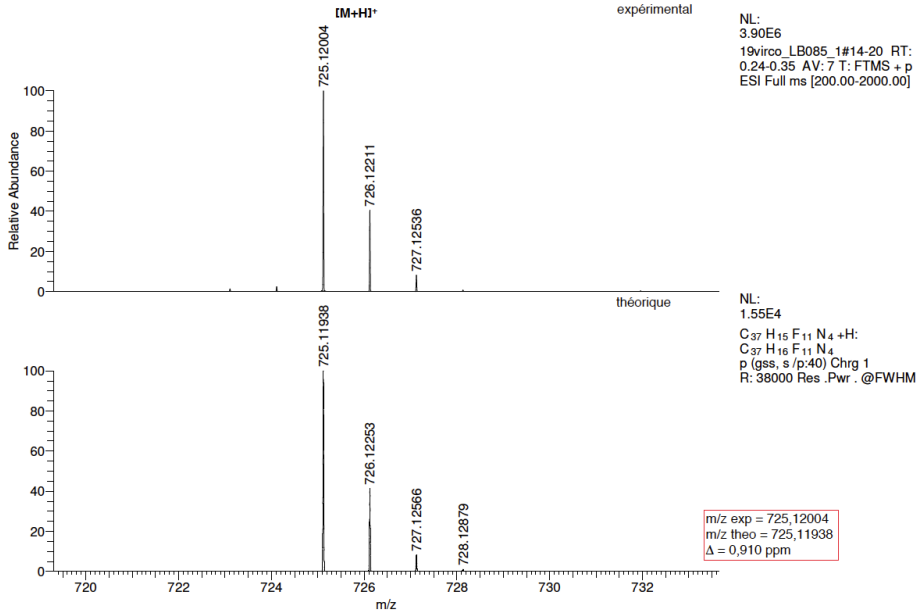
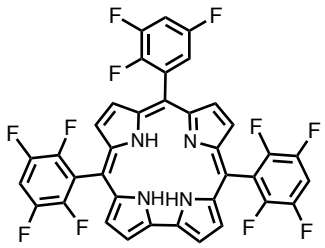


Figure S49: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pentafluorophenyl)corrole **17**.







Chemical Formula: $C_{37}H_{15}F_{11}N_4$
Exact Mass: 724.1121
Molecular Weight: 724.5374

Figure S50: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2',3',5'-trifluorophenyl)corrole **18**.

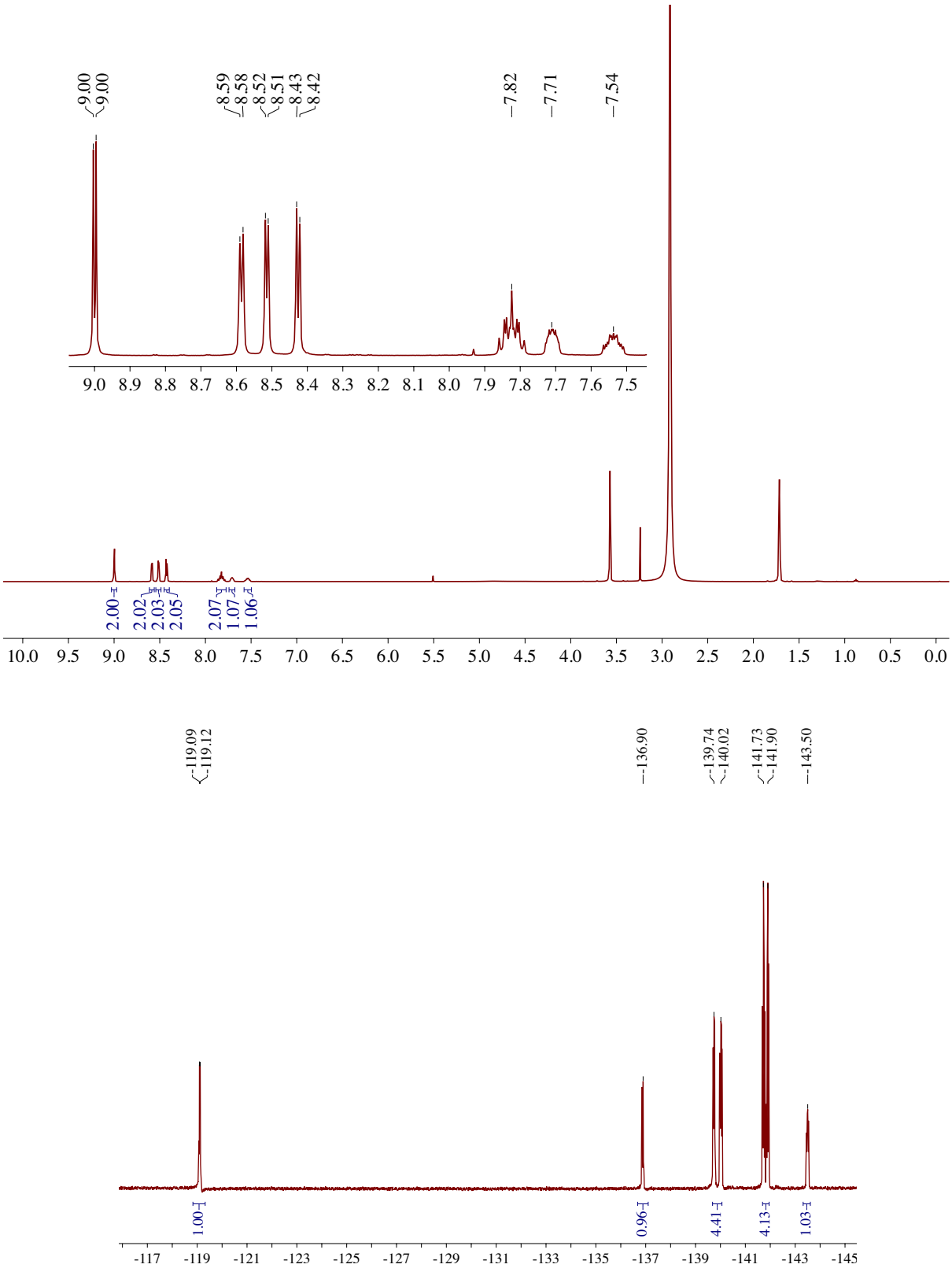


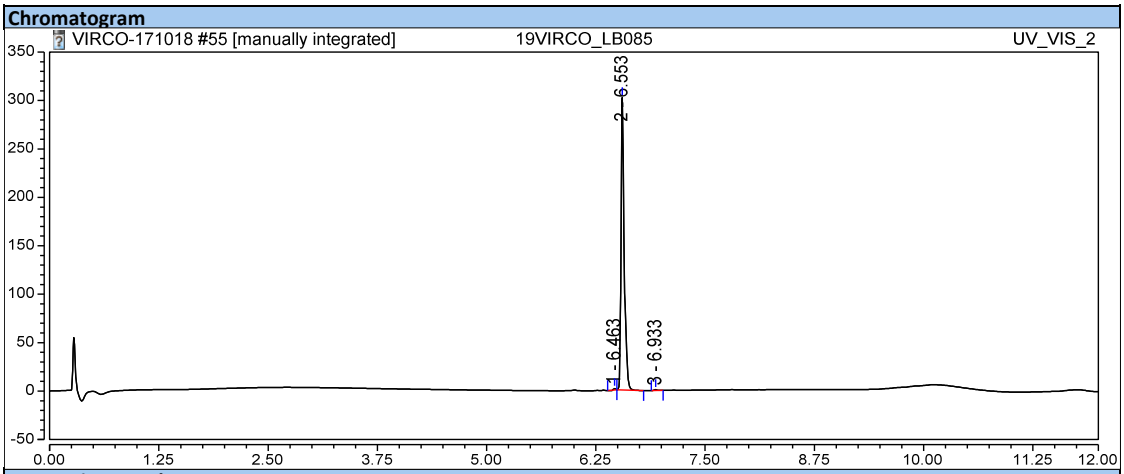
Figure S51: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2',3',5'-trifluorophenyl)corrole **18** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

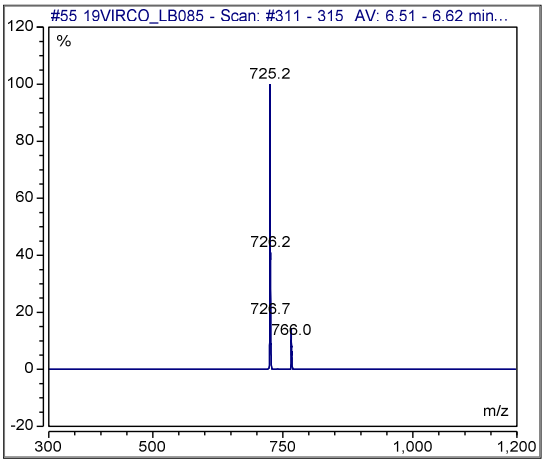
Injection Name:	**19VIRCO_LB085**	*Run Time (min):*	**12.00**
Vial Number:	**GB7**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**04/Apr/19 18:45**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.463	0.031	1.720	0.24	0.56	n.a.
2		6.553	12.745	301.850	99.49	99.13	n.a.
3		6.933	0.035	0.942	0.27	0.31	n.a.
Total:			**12.810**	**304.512**	**100.00**	**100.00**	



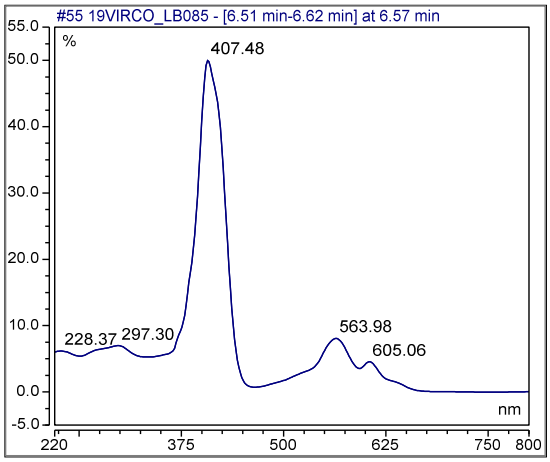
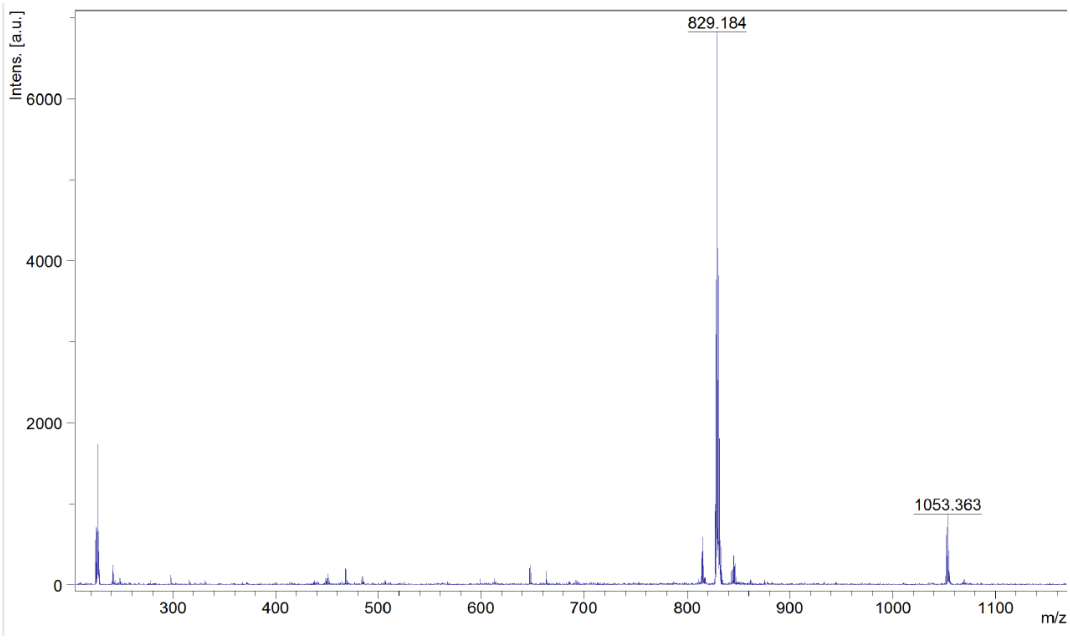
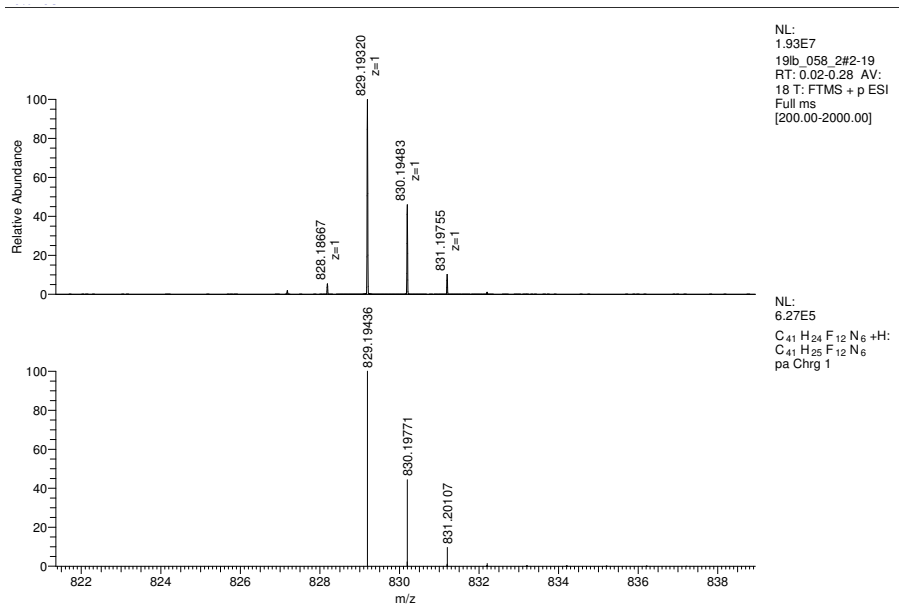
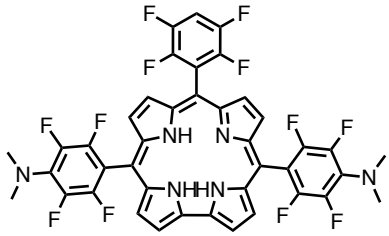


Figure S52: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2',3',5'-trifluorophenyl)corrole **18**.







Chemical Formula: $C_{41}H_{24}F_{12}N_6$
Exact Mass: 828.1871
Molecular Weight: 828.6658

Figure S53: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(4'-(dimethylamino)-2',3',5',6'-tetrafluorophenyl)-10-(2',3',5',6'-tetrafluorophenyl)corrole **19**.

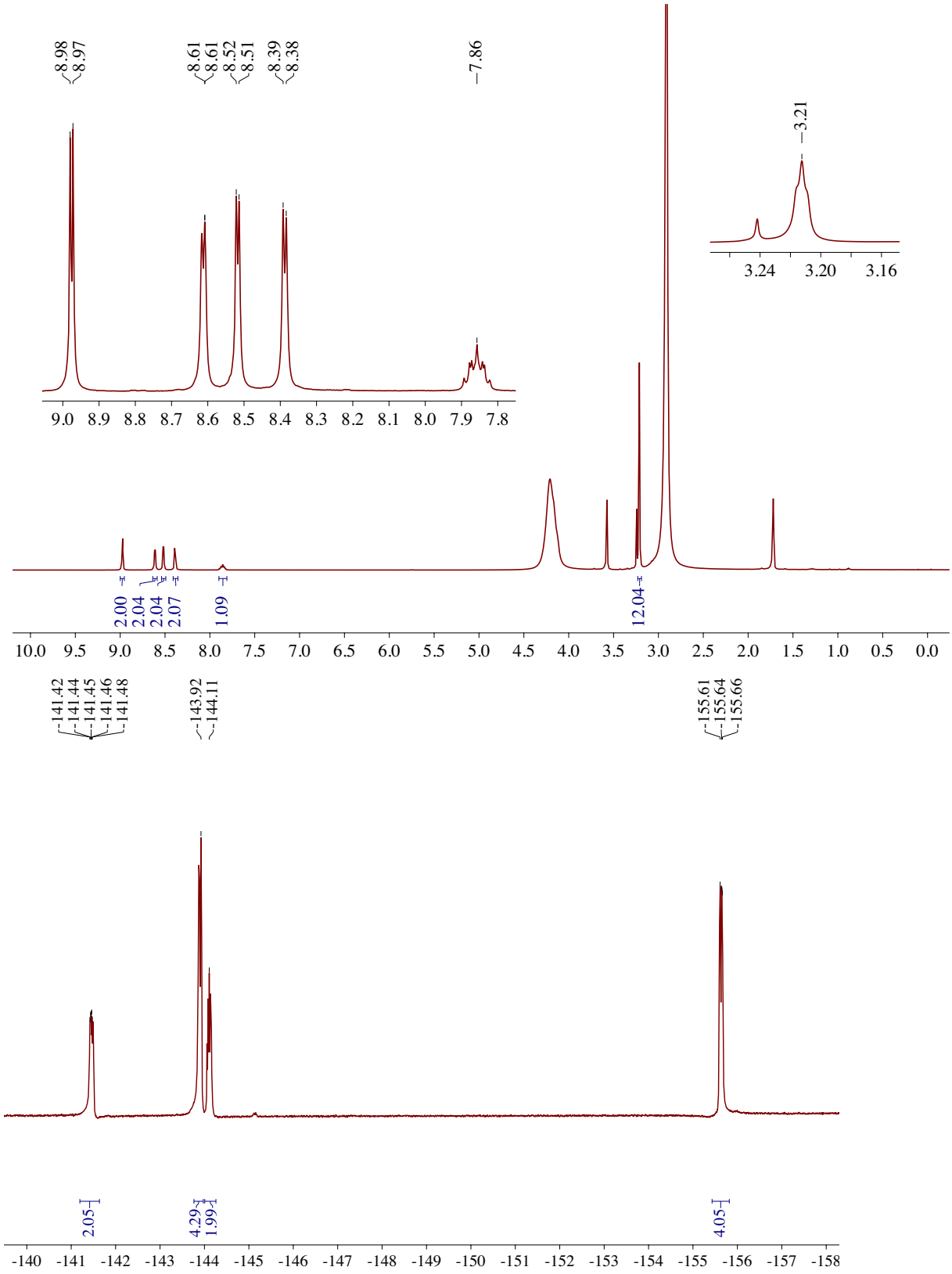


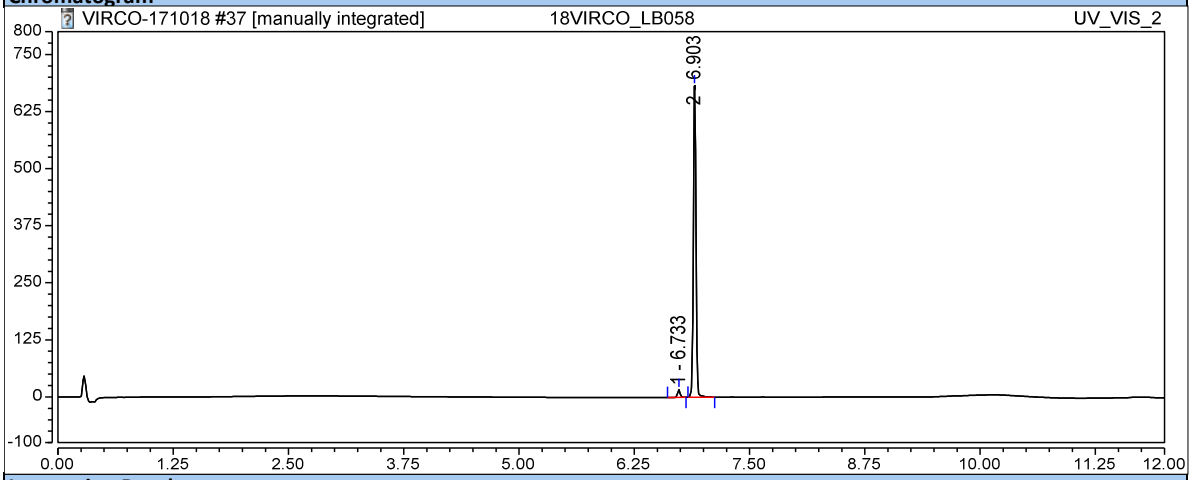
Figure S54: ^{1}H NMR (top) and ^{19}F spectra (down) of 5,15-bis(4'-(dimethylamino)-2',3',5',6'-tetrafluorophenyl)-10-(2',3',5',6'-tetrafluorophenyl)corrole **19** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

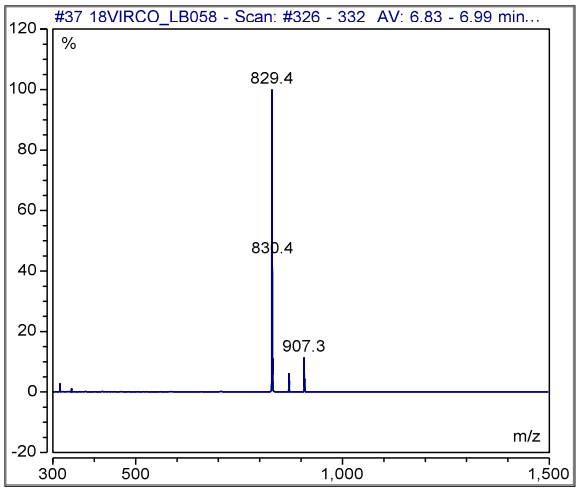
Injection Name:	**18VIRCO_LB058**	*Run Time (min):*	**12.00**
Vial Number:	**BA6**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**28/Feb/19 16:13**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.733	0.543	16.997	2.35	2.43	n.a.
2		6.903	22.572	681.702	97.65	97.57	n.a.
Total:			**23.115**	**698.699**	**100.00**	**100.00**	



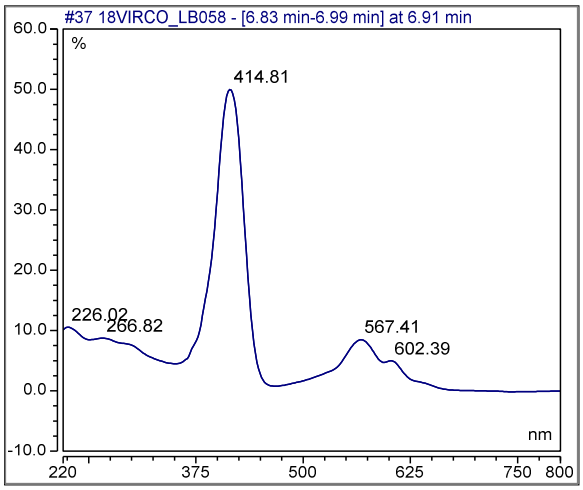
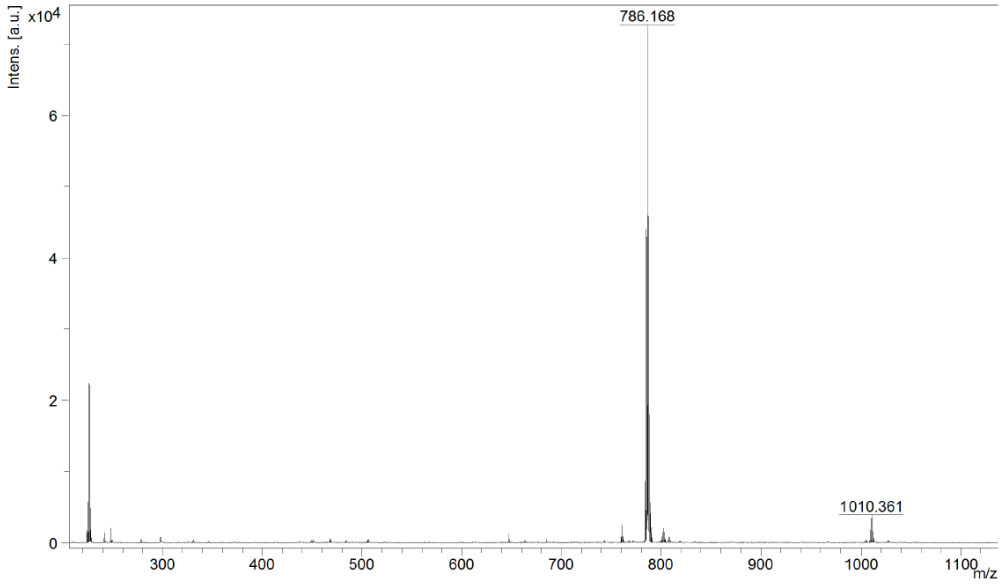
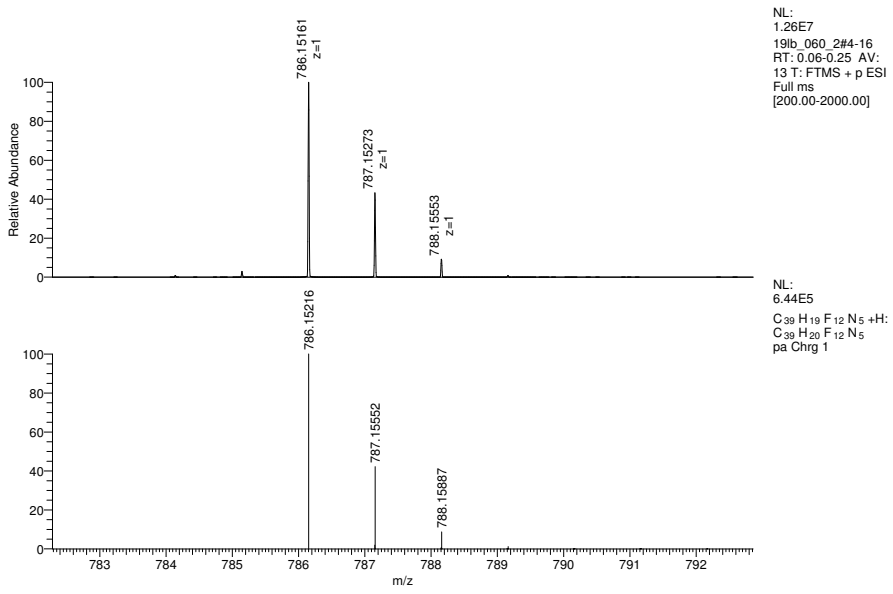
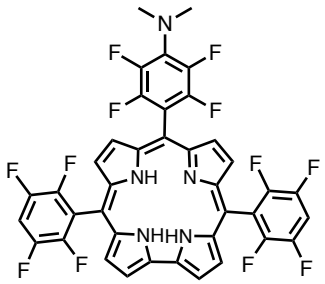


Figure S55: HPLC chromatogram of 5,15-bis(4'-(dimethylamino)-2',3',5',6'-tetrafluorophenyl)-10-(2',3',5',6'-tetrafluorophenyl)corrole **19**.







Chemical Formula: $C_{39}H_{19}F_{12}N_5$
Exact Mass: 785.1449
Molecular Weight: 785.5968

Figure S56: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(4'-(dimethylamino)-2',3',5',6'-tetrafluorophenyl)corrole **20**.

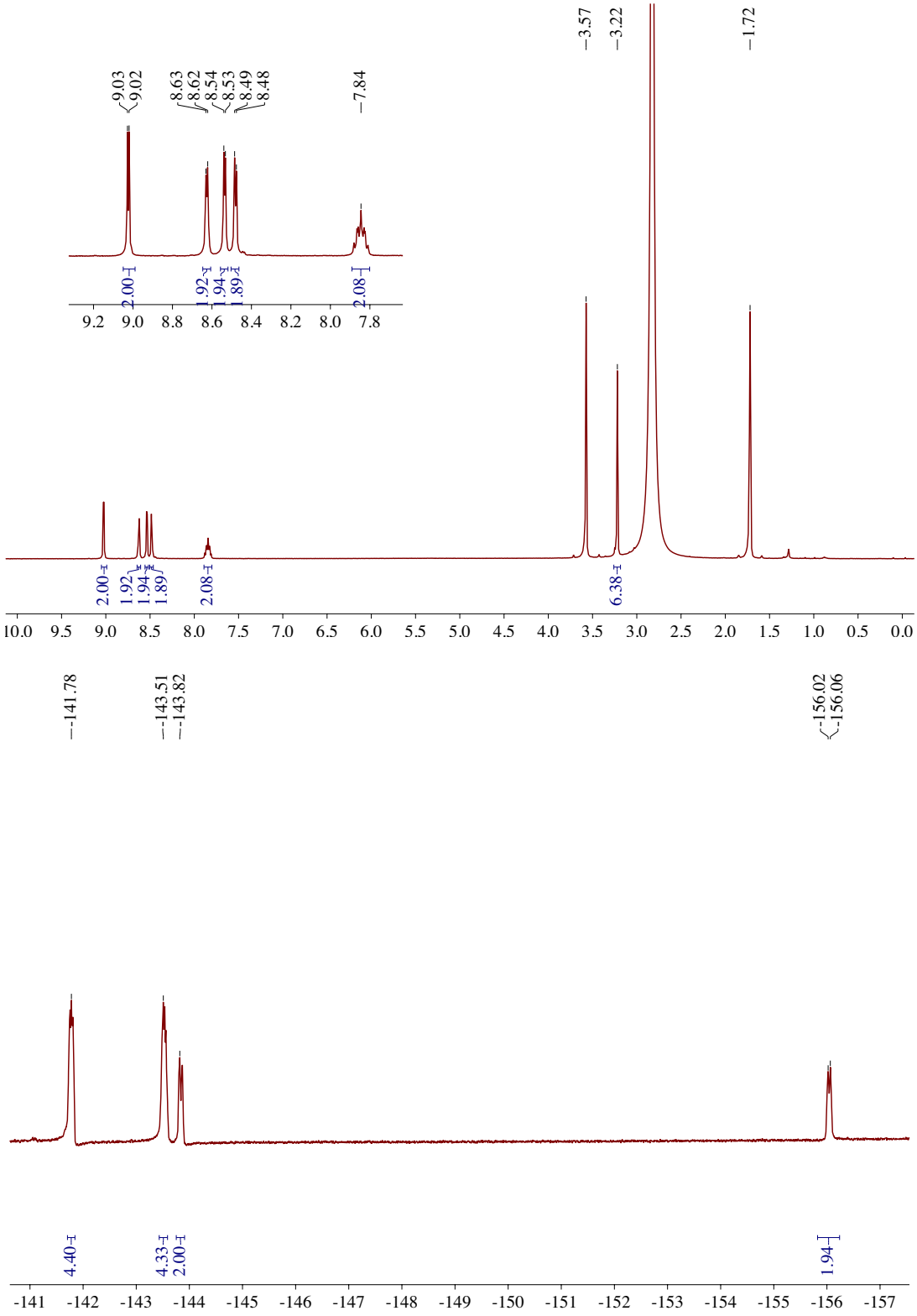


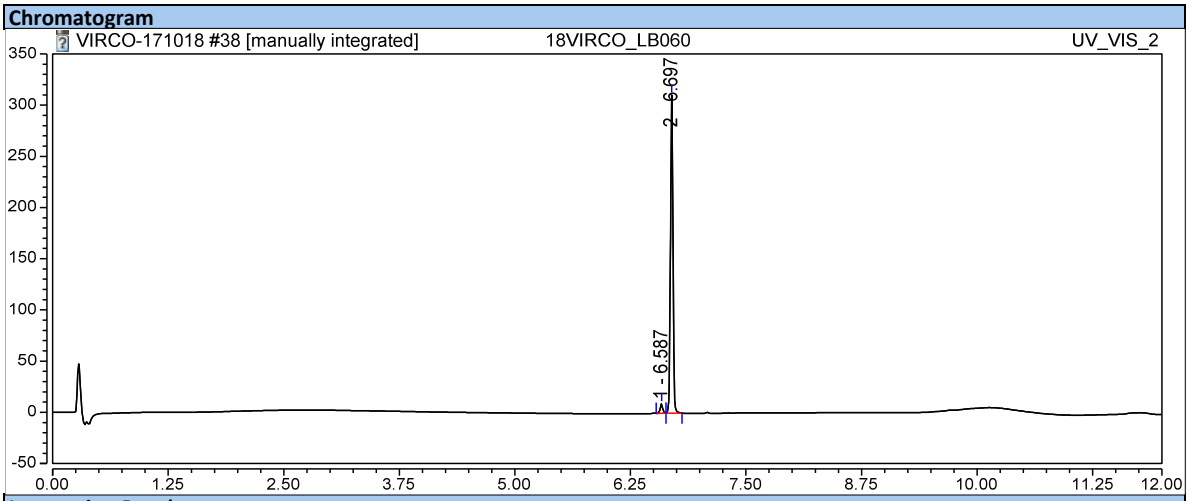
Figure S57: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(4'-(dimethylamino)-2',3',5',6'-tetrafluorophenyl)corrole **20** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

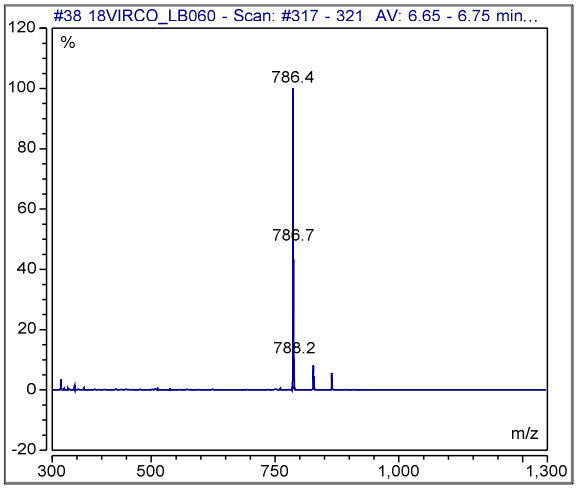
Injection Name:	**18VIRCO_LB060**	*Run Time (min):*	**12.00**
Vial Number:	**BA7**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**28/Feb/19 16:27**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.587	0.272	9.116	2.66	2.85	n.a.
2		6.697	9.953	310.503	97.34	97.15	n.a.
Total:			**10.224**	**319.619**	**100.00**	**100.00**	



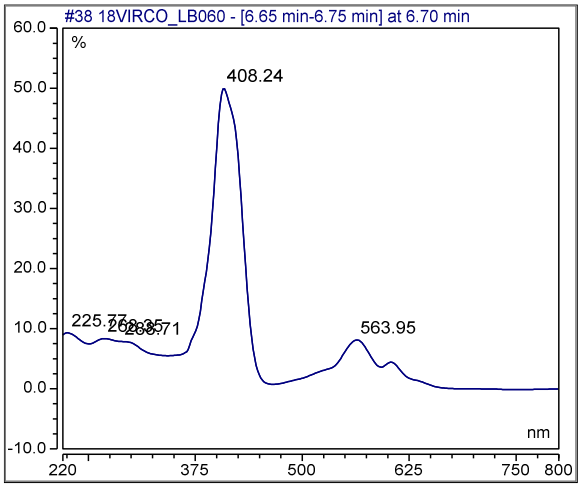
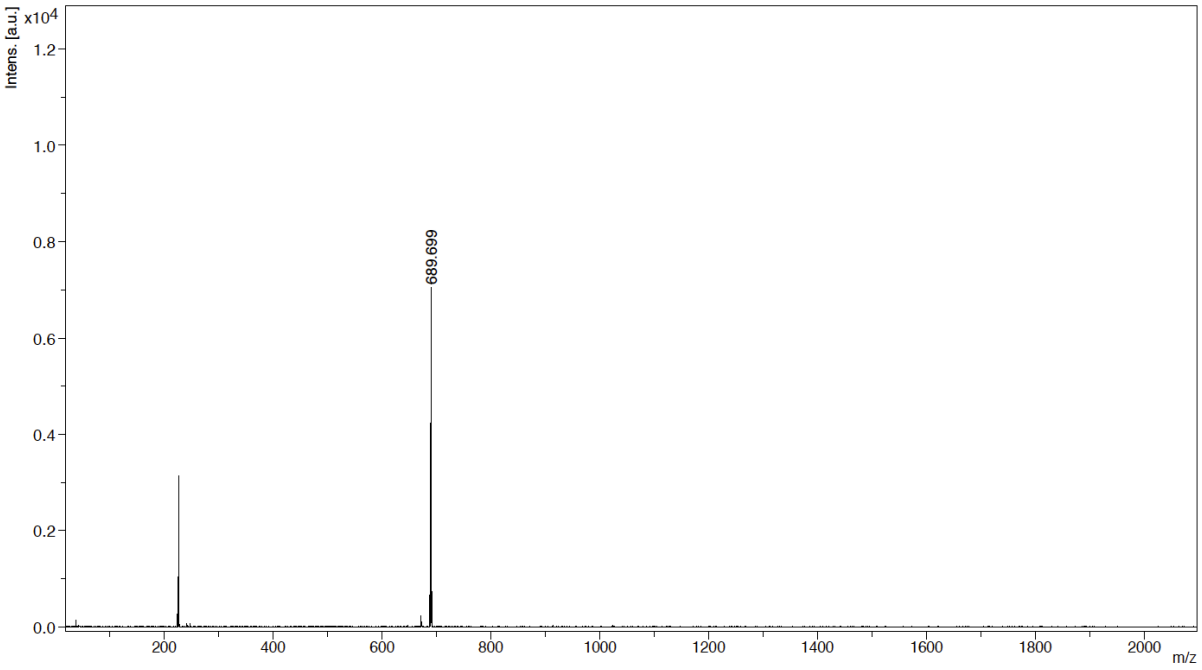
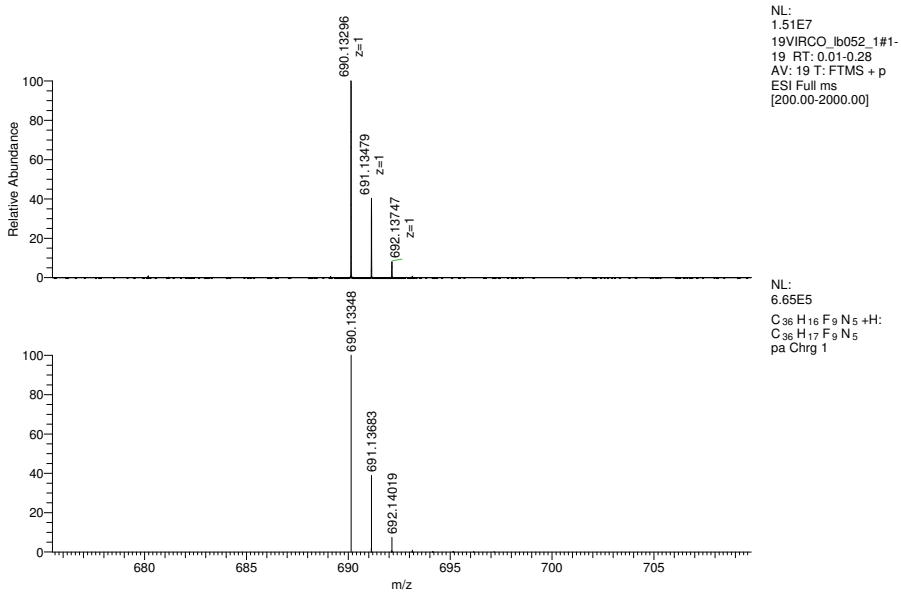
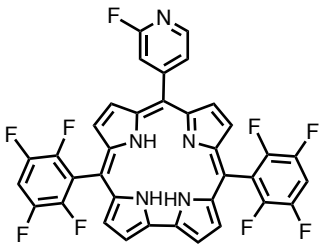


Figure S58: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(4'-(dimethylamino)-2',3',5',6'-tetrafluorophenyl)corrole **20**.







Chemical Formula: $C_{36}H_{16}F_9N_5$
Exact Mass: 689.1262
Molecular Weight: 689.5446

Figure S59: MALDI/TOF LRMS and HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2'-fluoropyrid-4'-yl)corrole **21**.

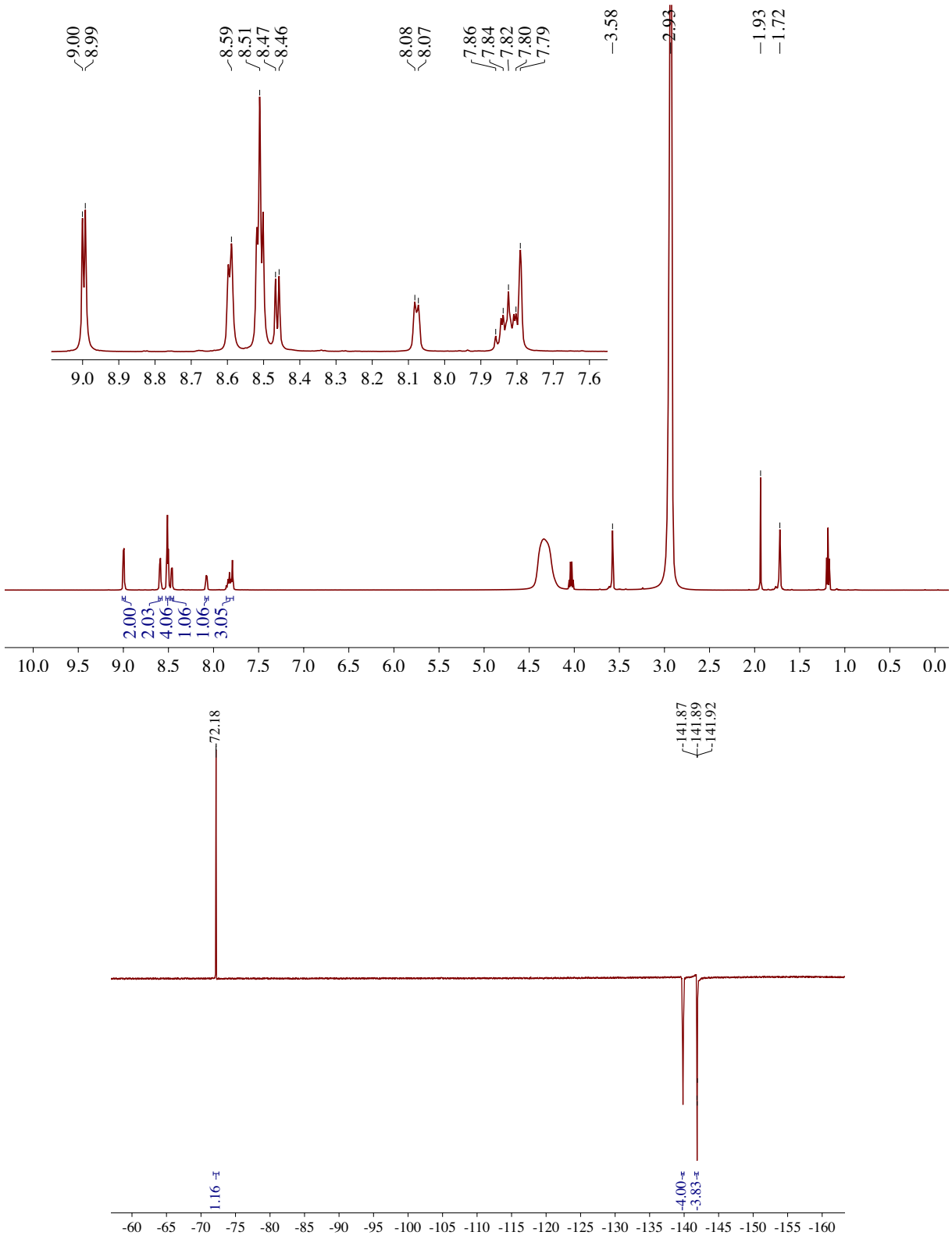


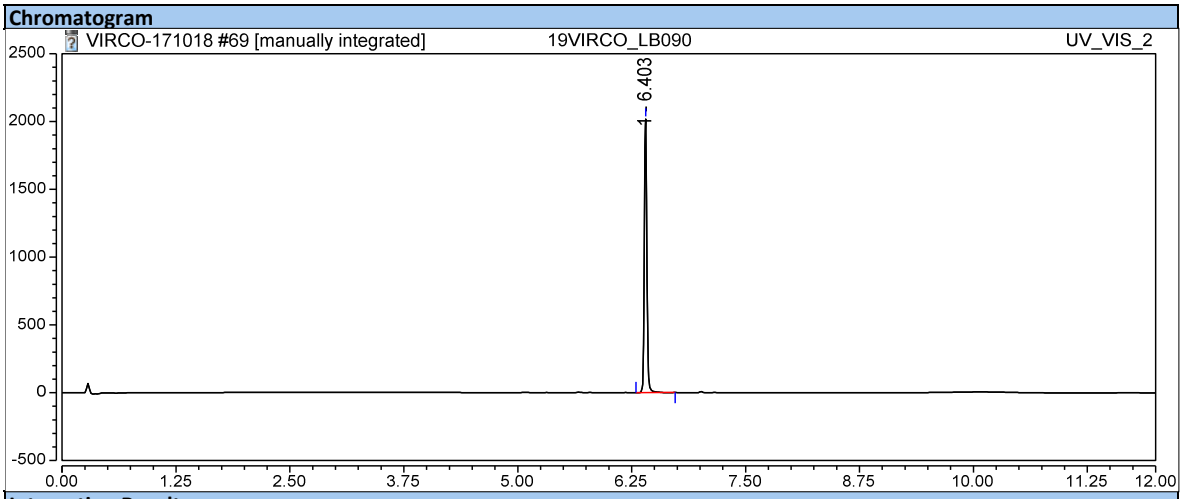
Figure S60: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2'-fluoropyrid-4'-yl)corrole **21** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

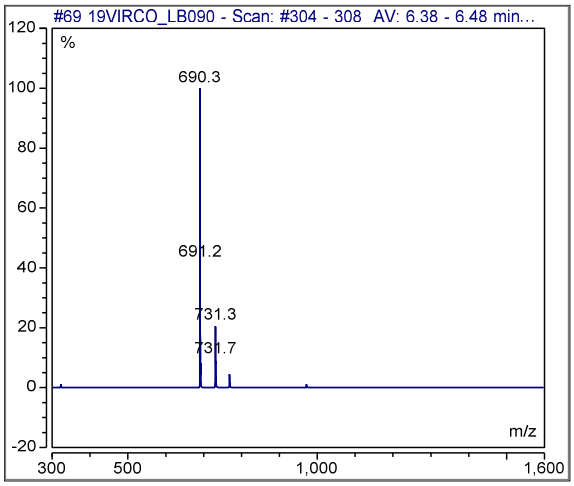
Injection Name:	**19VIRCO_LB090**	*Run Time (min):*	**12.00**
Vial Number:	**RC4**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**30/Apr/19 17:23**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.403	65.962	2017.553	100.00	100.00	n.a.
Total:			**65.962**	**2017.553**	**100.00**	**100.00**	



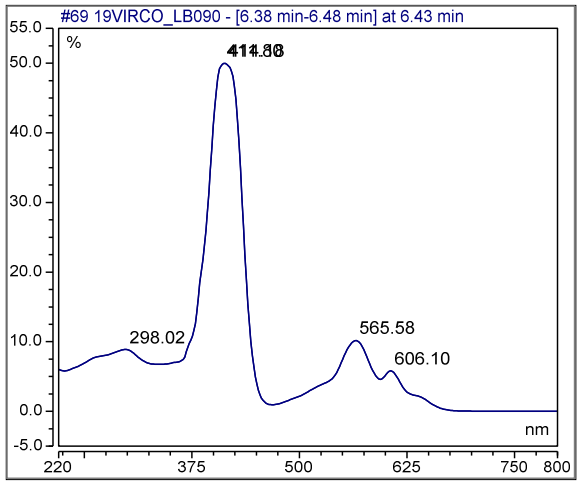
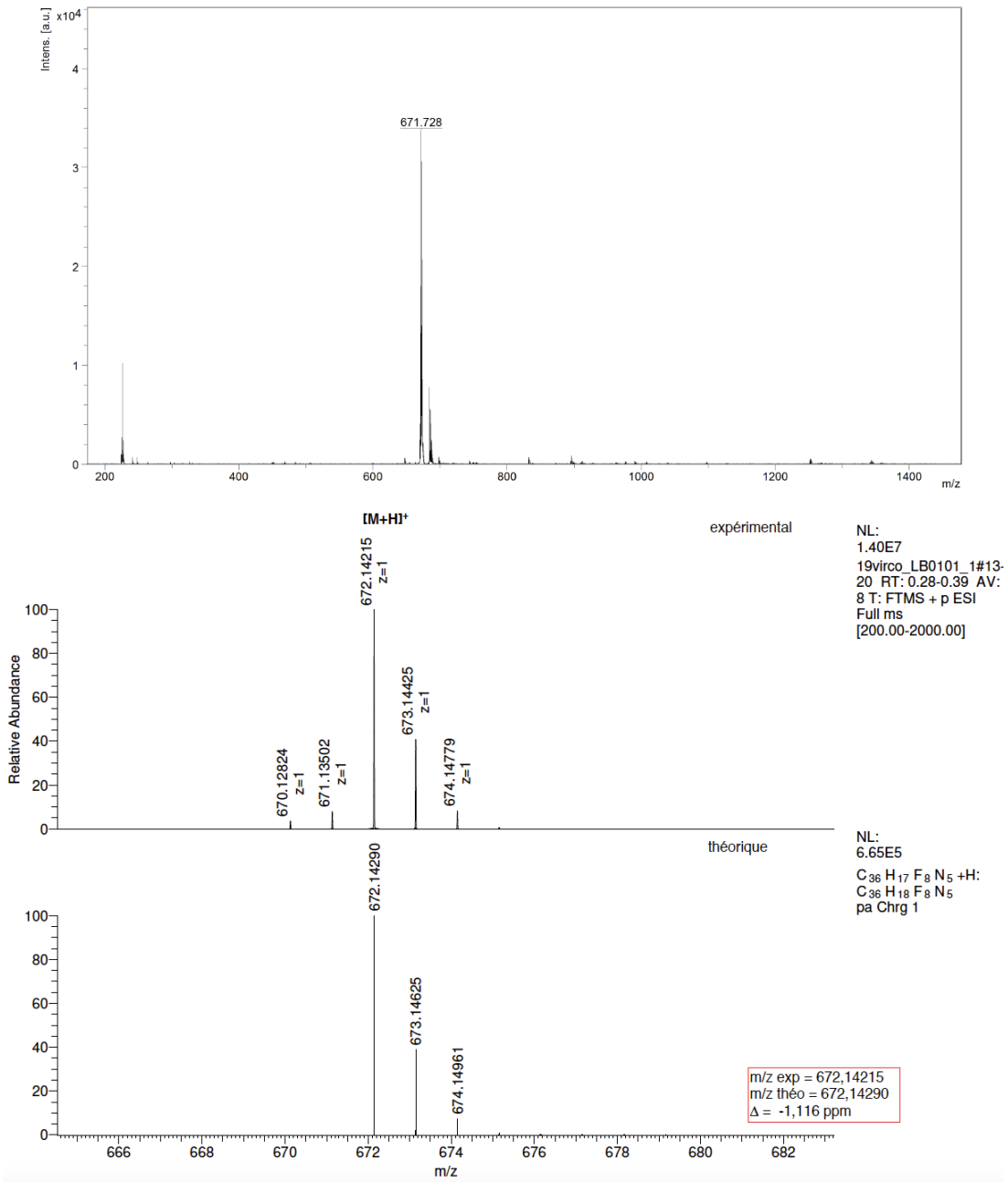
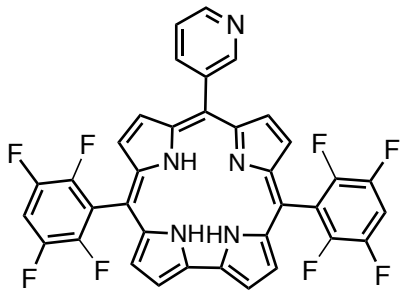


Figure S61: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2'-fluoropyrid-4'-yl)corrole **21**.





Chemical Formula: $C_{36}H_{17}F_8N_5$

Exact Mass: 671.1356

Molecular Weight: 671.5542

Figure S62: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pyrid-3'-yl)corrole **22**.

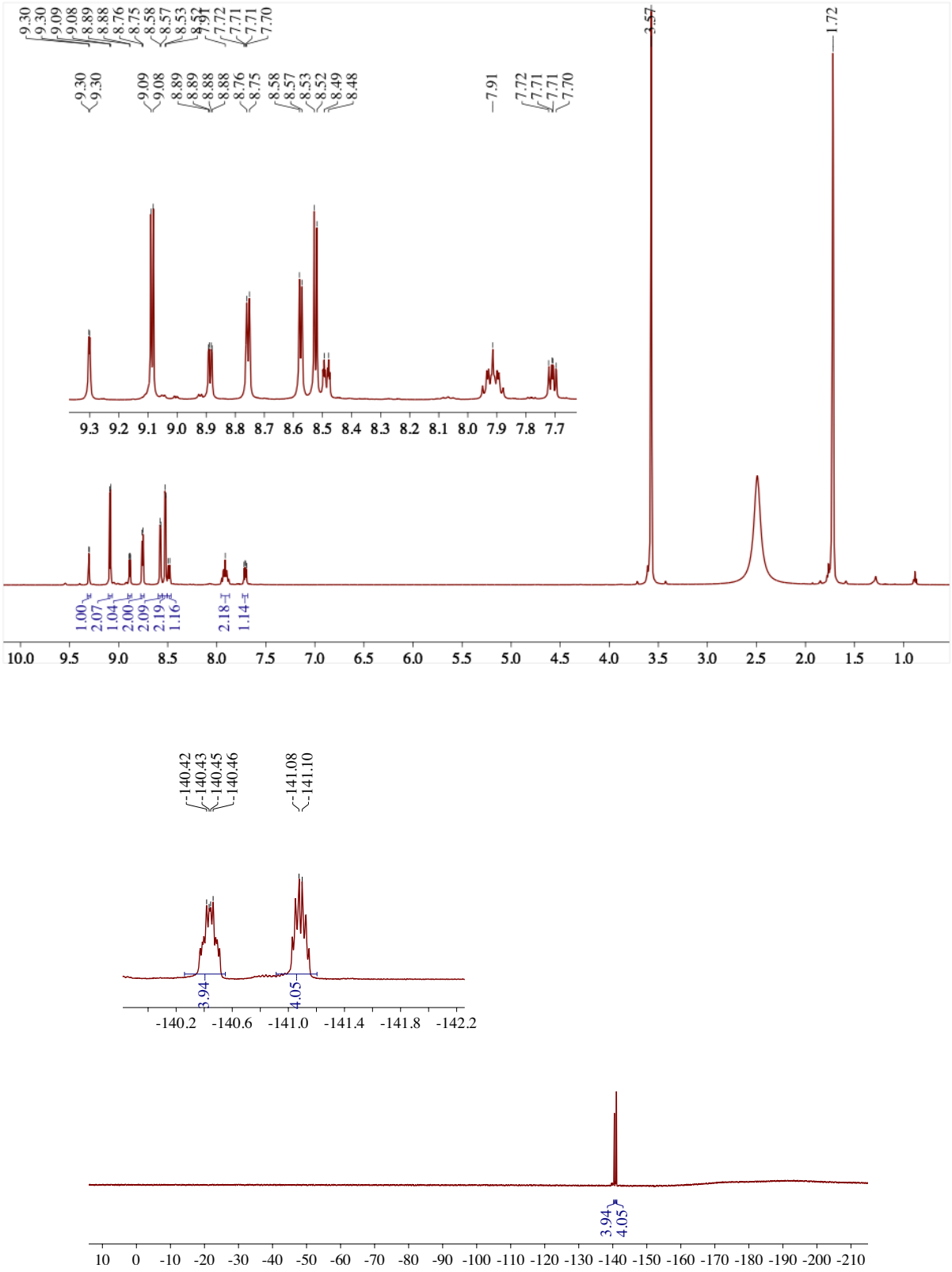


Figure S63: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pyrid-3'-yl)corrole **22** in THF-d_8 + one drop of hydrazine hydrate 64%.

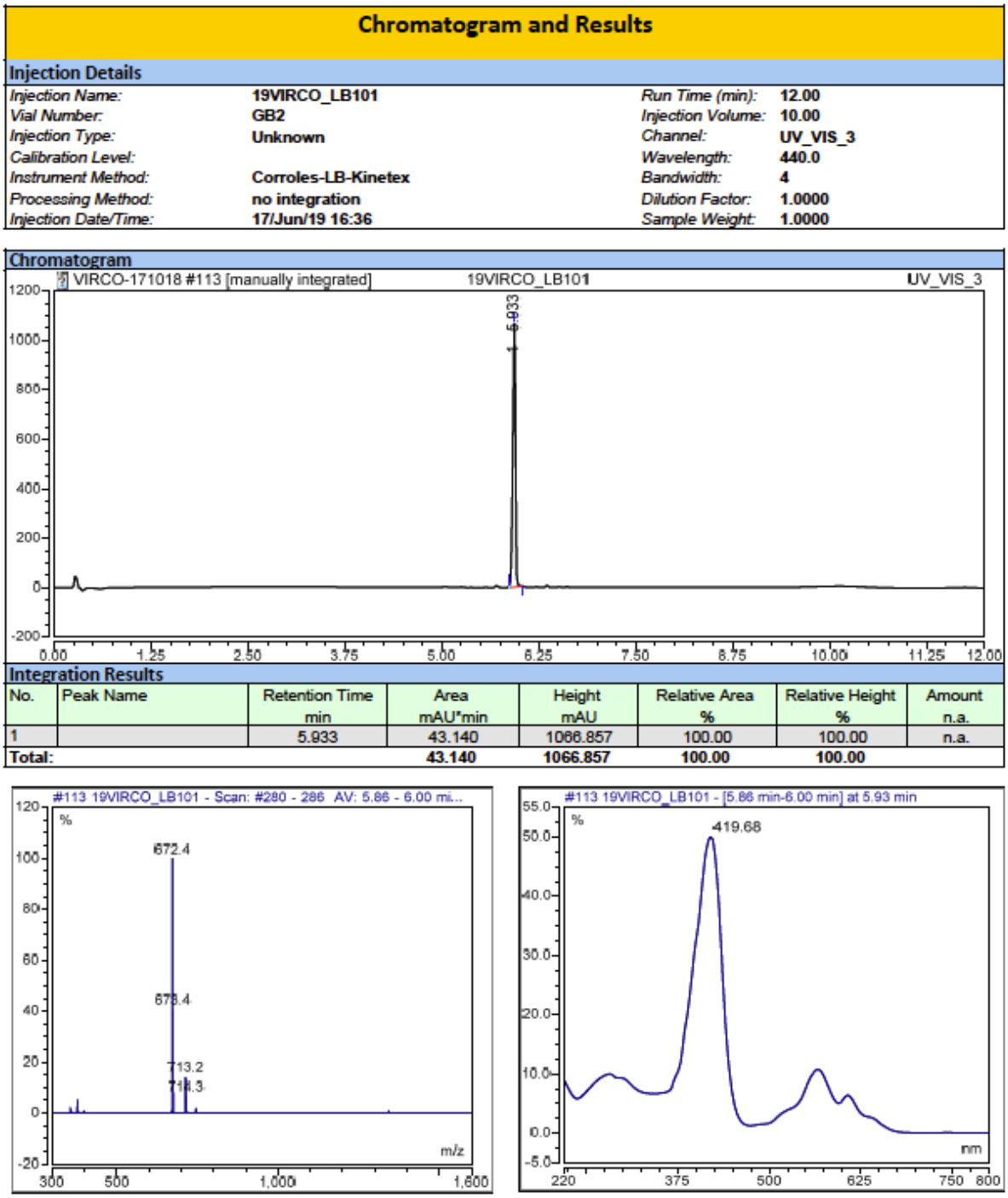
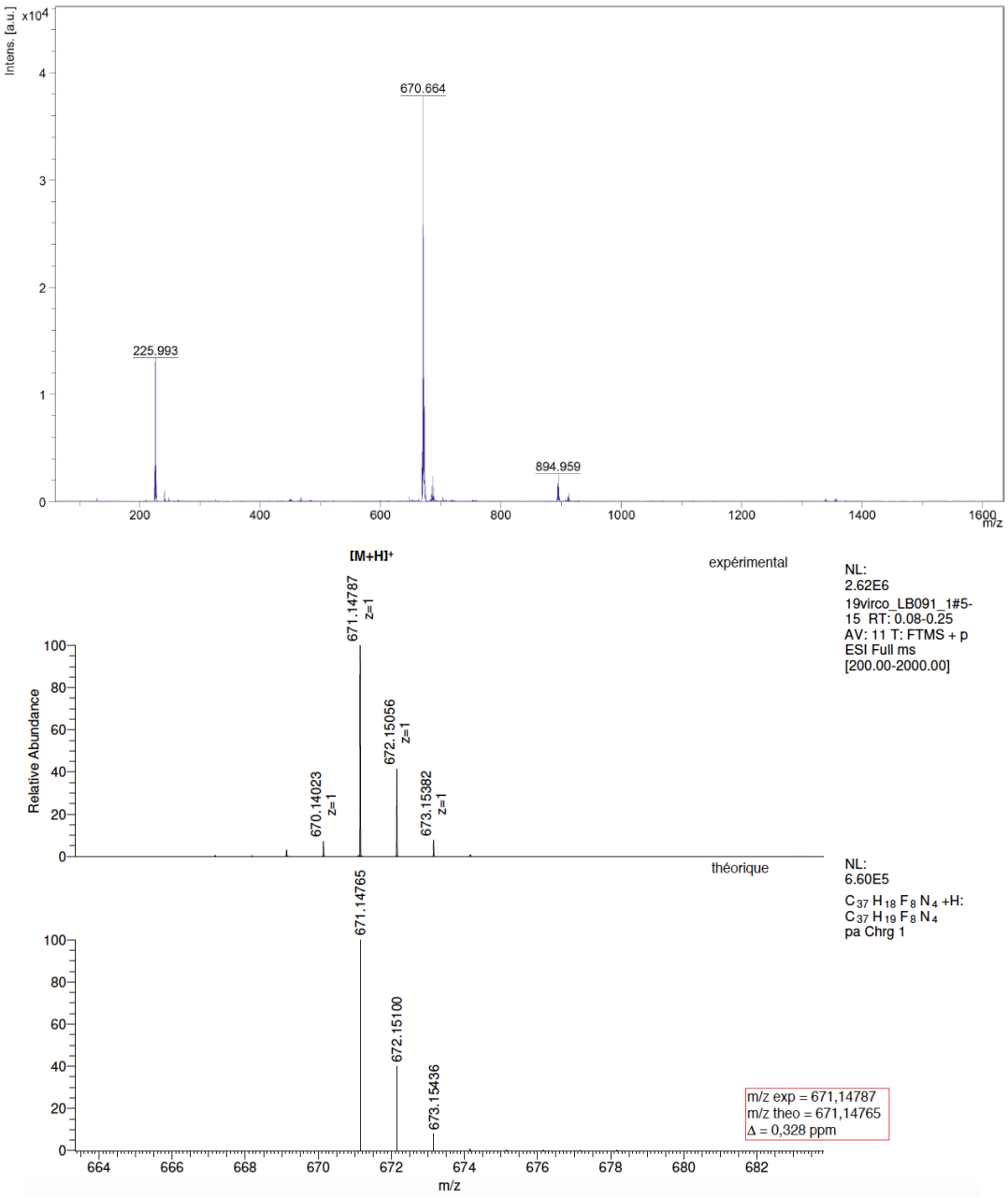
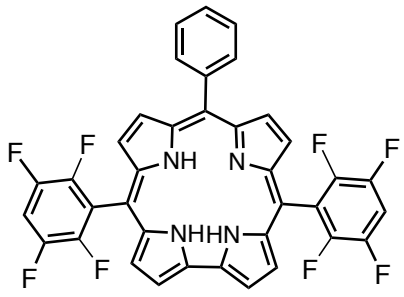


Figure S64: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pyrid-3'-yl)corrole **22**.





Chemical Formula: $C_{37}H_{18}F_8N_4$

Exact Mass: 670.1404

Molecular Weight: 670.5662

Figure S65: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-phenylcorrole **23**.

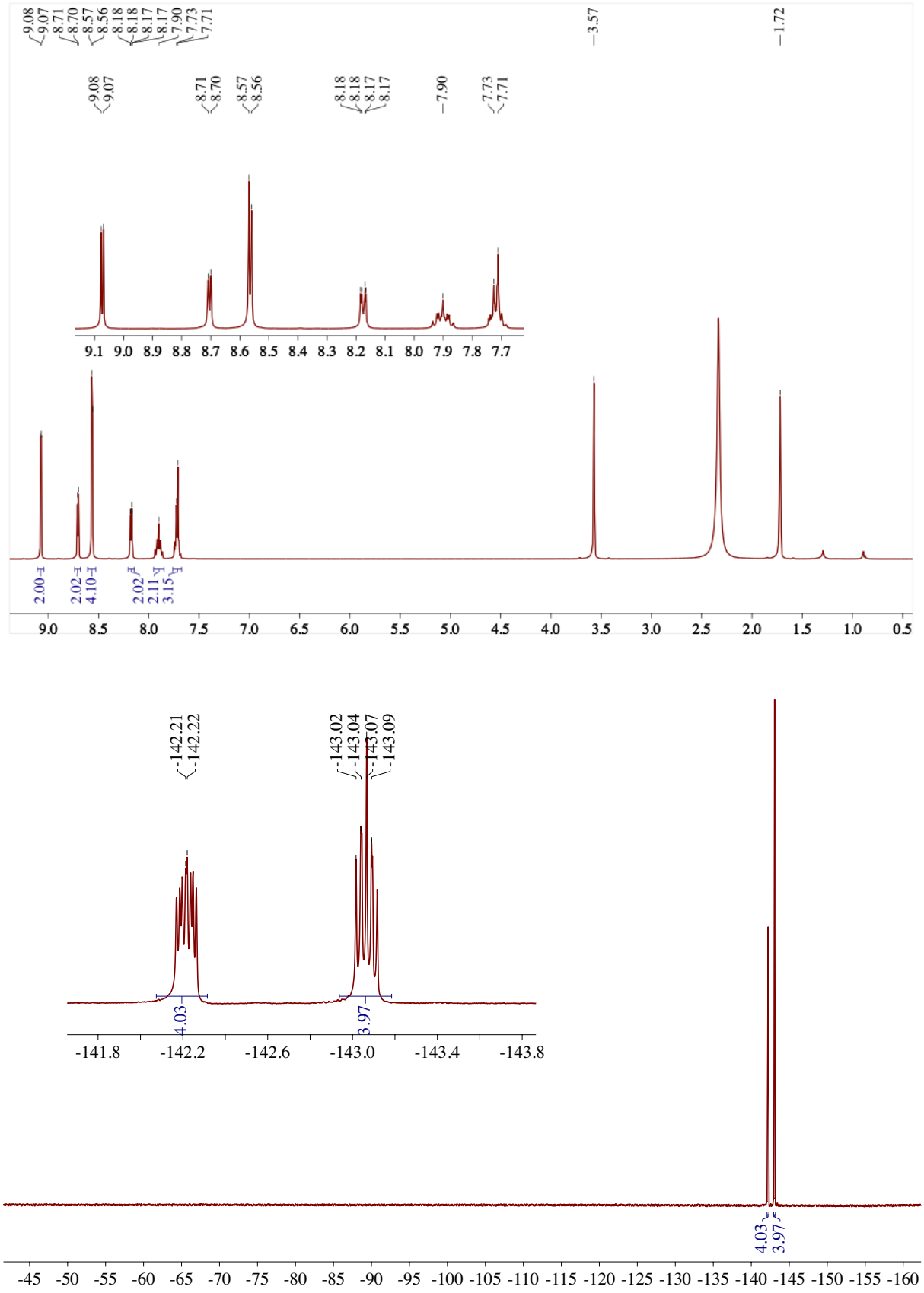


Figure S66: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-phenylcorrole **23** in THF-d_8 + one drop of hydrazine hydrate 64%.

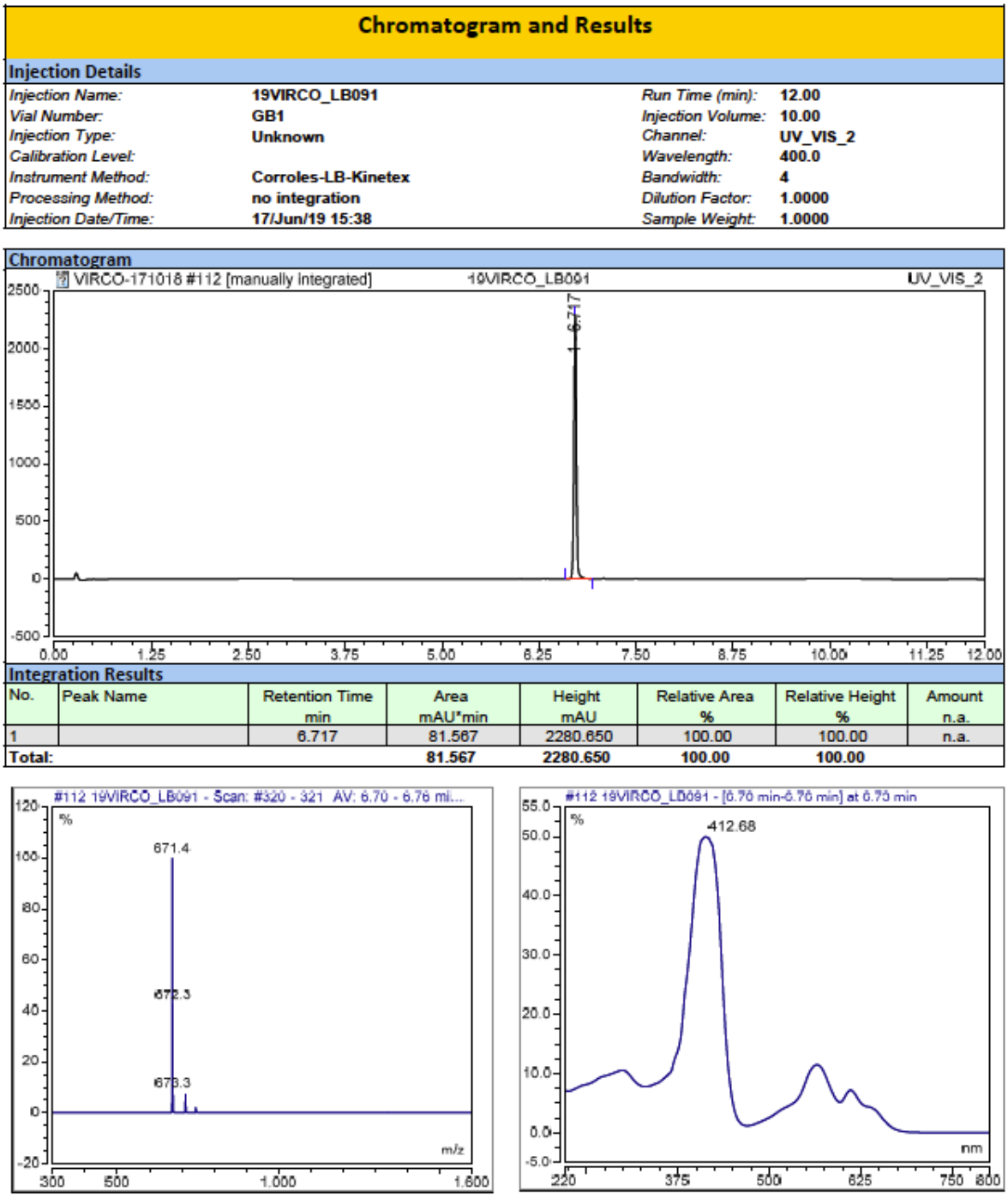
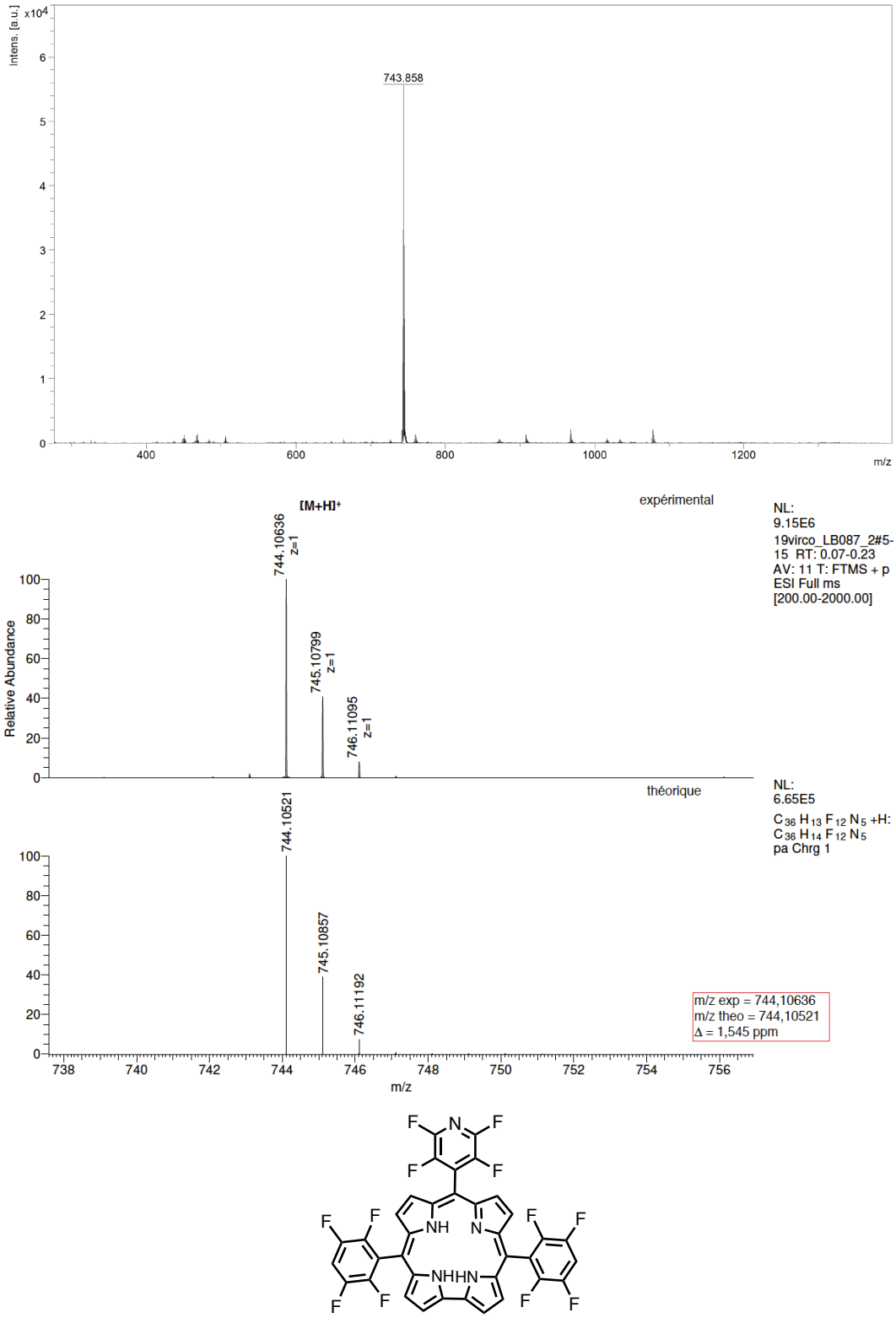


Figure S67: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-phenylcorrole **23.**



Chemical Formula: $C_{36}H_{13}F_{12}N_5$

Exact Mass: 743.0979

Molecular Weight: 743.515

Figure S68: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2',3',5',6'-tetrafluoro-pyrid-4'-yl)corrole **24**.

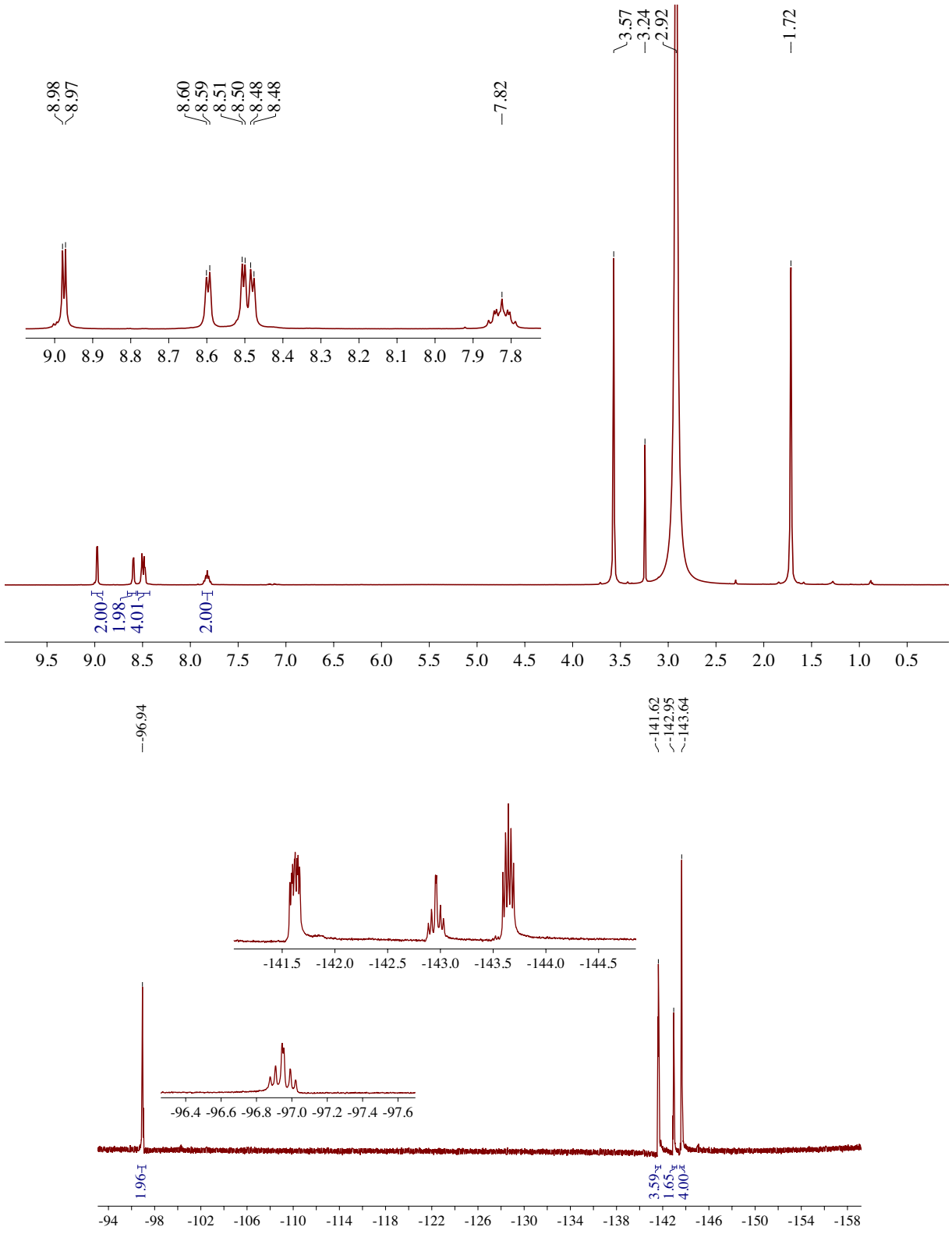


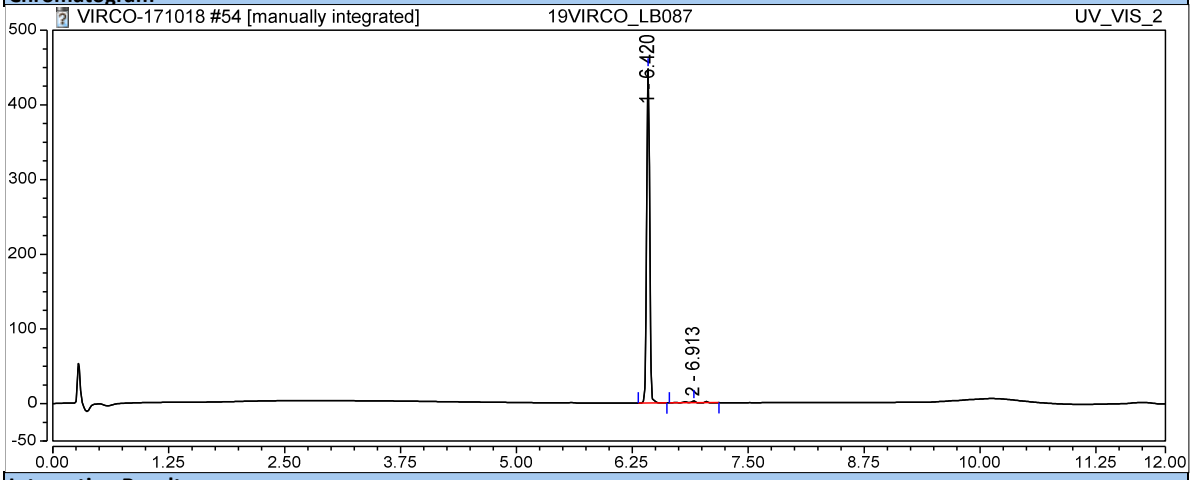
Figure S69: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2',3',5',6'-tetrafluoro-pyrid-4'-yl)corrole **24** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

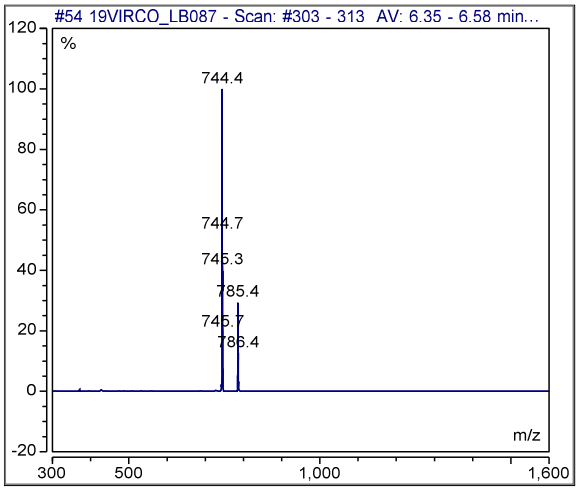
Injection Name:	**19VIRCO_LB087**	*Run Time (min):*	**12.00**
Vial Number:	**BC4**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**28/Mar/19 15:11**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.420	16.980	447.147	98.49	99.40	n.a.
2		6.913	0.260	2.684	1.51	0.60	n.a.
Total:			**17.241**	**449.831**	**100.00**	**100.00**	



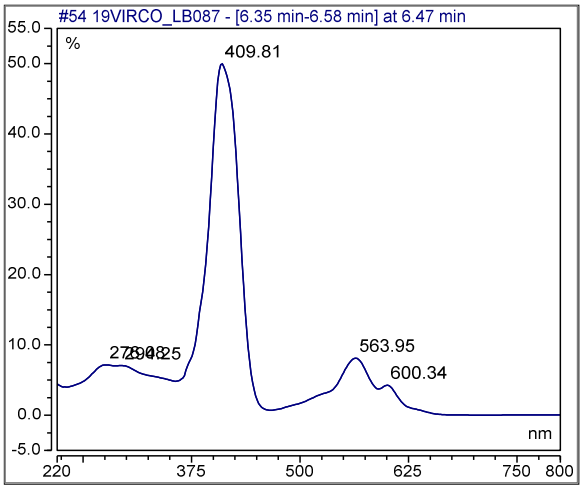
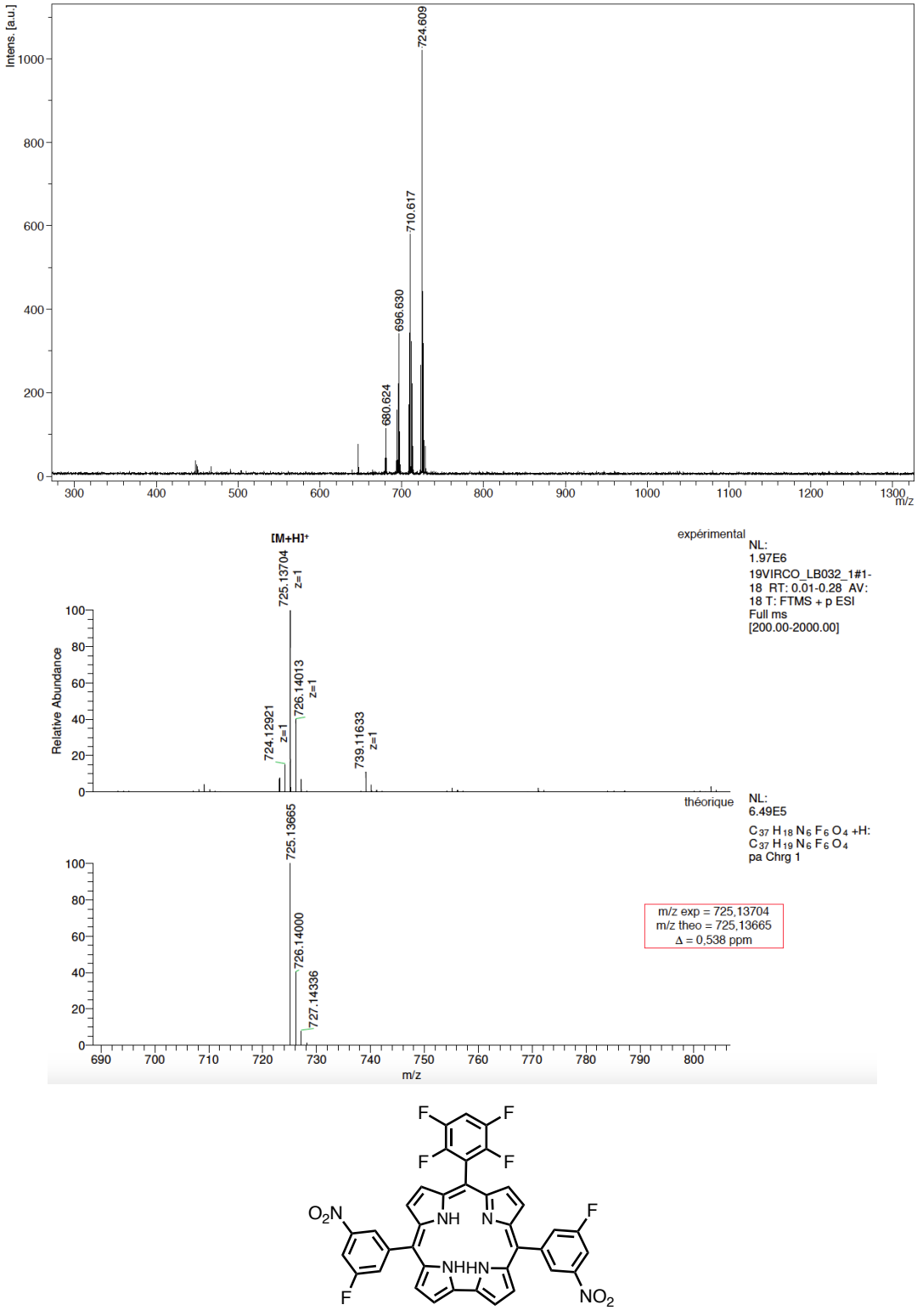


Figure S70: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(2',3',5',6'-tetrafluoro-pyrid-4'-yl)corrole **24**.



Chemical Formula: $C_{37}H_{18}F_6N_6O_4$
Exact Mass: 724.1294
Molecular Weight: 724.5794

Figure S71: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(3'-fluoro-5'-nitrophenyl)-10-(2',3',5',6'-tetrafluorophenyl)corrole **25**.

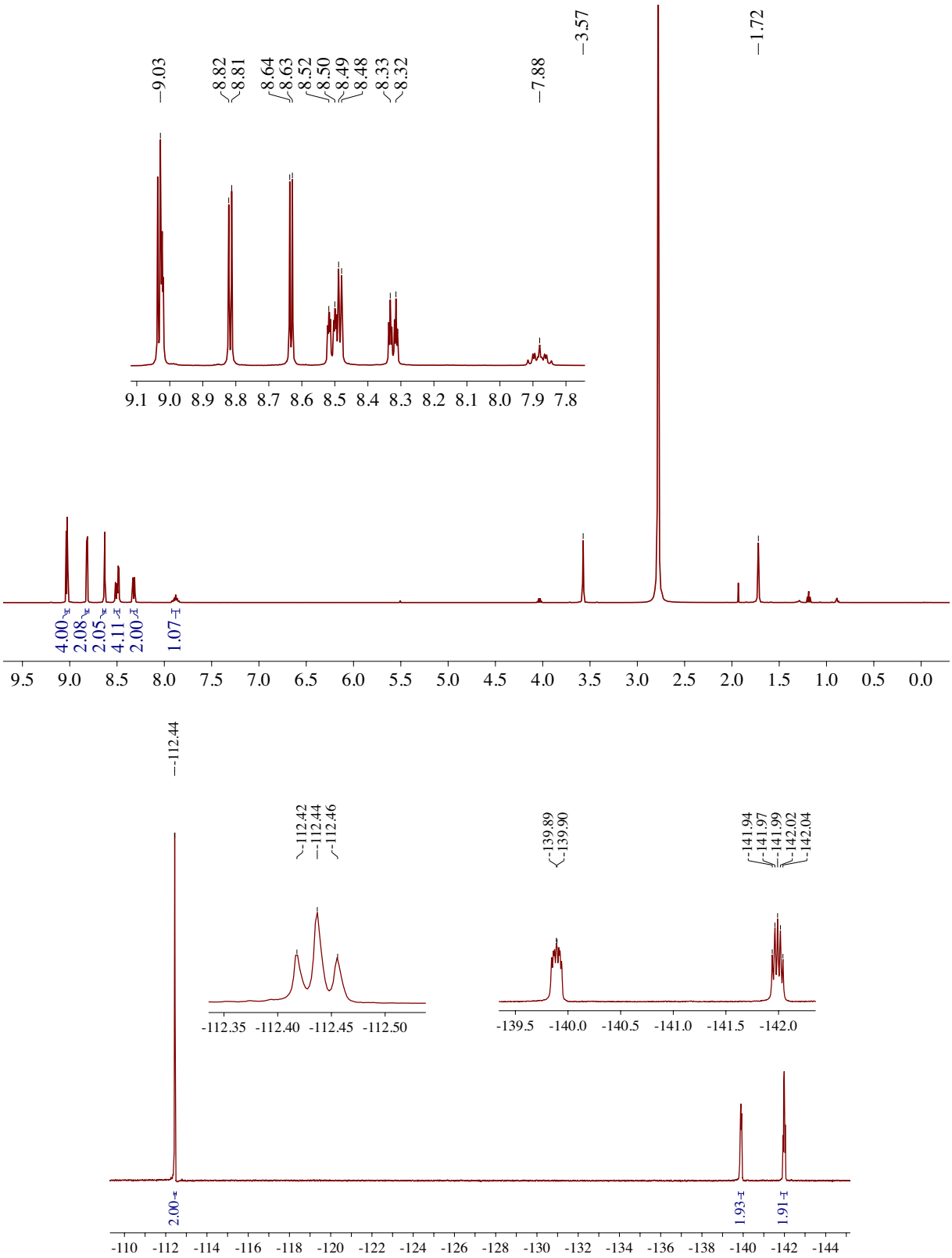


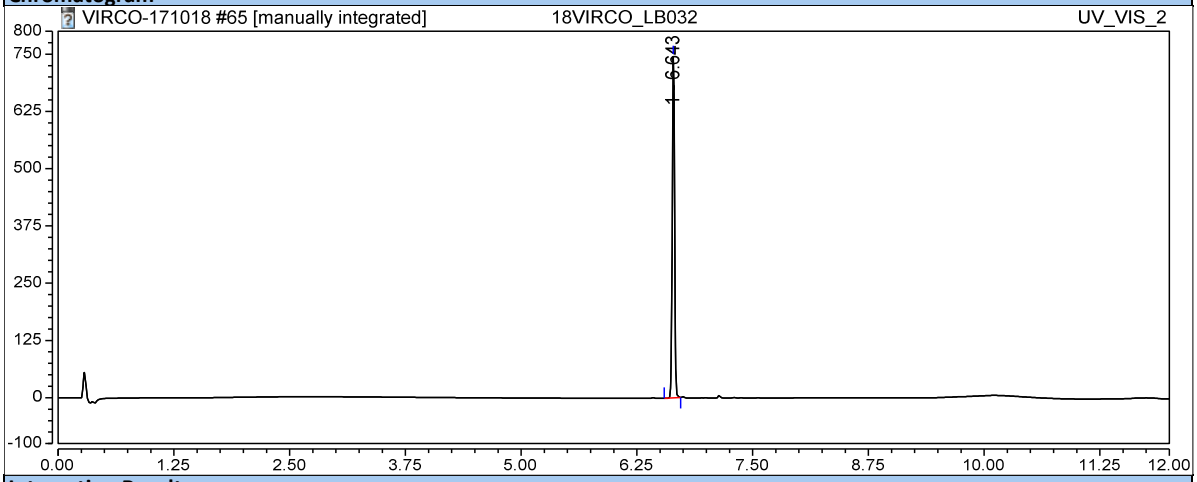
Figure S72: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(3'-fluoro-5'-nitrophenyl)-10-(2',3',5',6'-tetrafluorophenyl)corrole **25** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

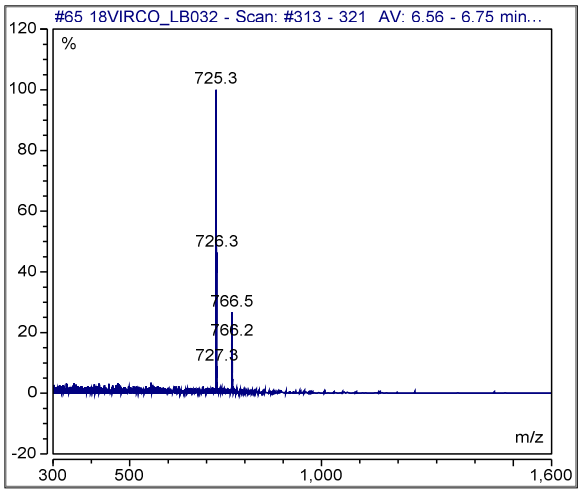
Injection Name:	**18VIRCO_LB032**	*Run Time (min):*	**12.00**
Vial Number:	**GD7**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**18/Apr/19 20:57**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.643	21.275	744.532	100.00	100.00	n.a.
Total:			**21.275**	**744.532**	**100.00**	**100.00**	



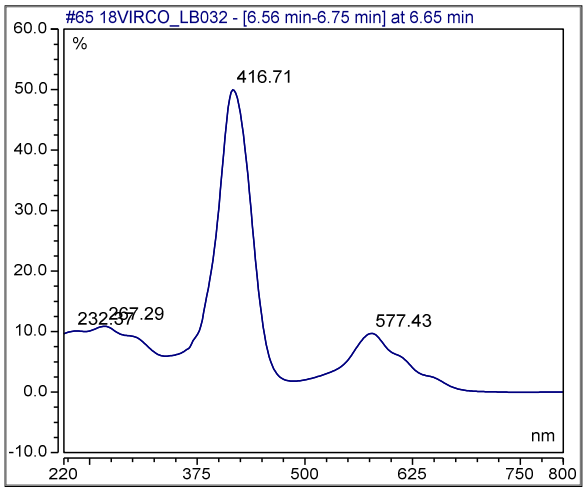
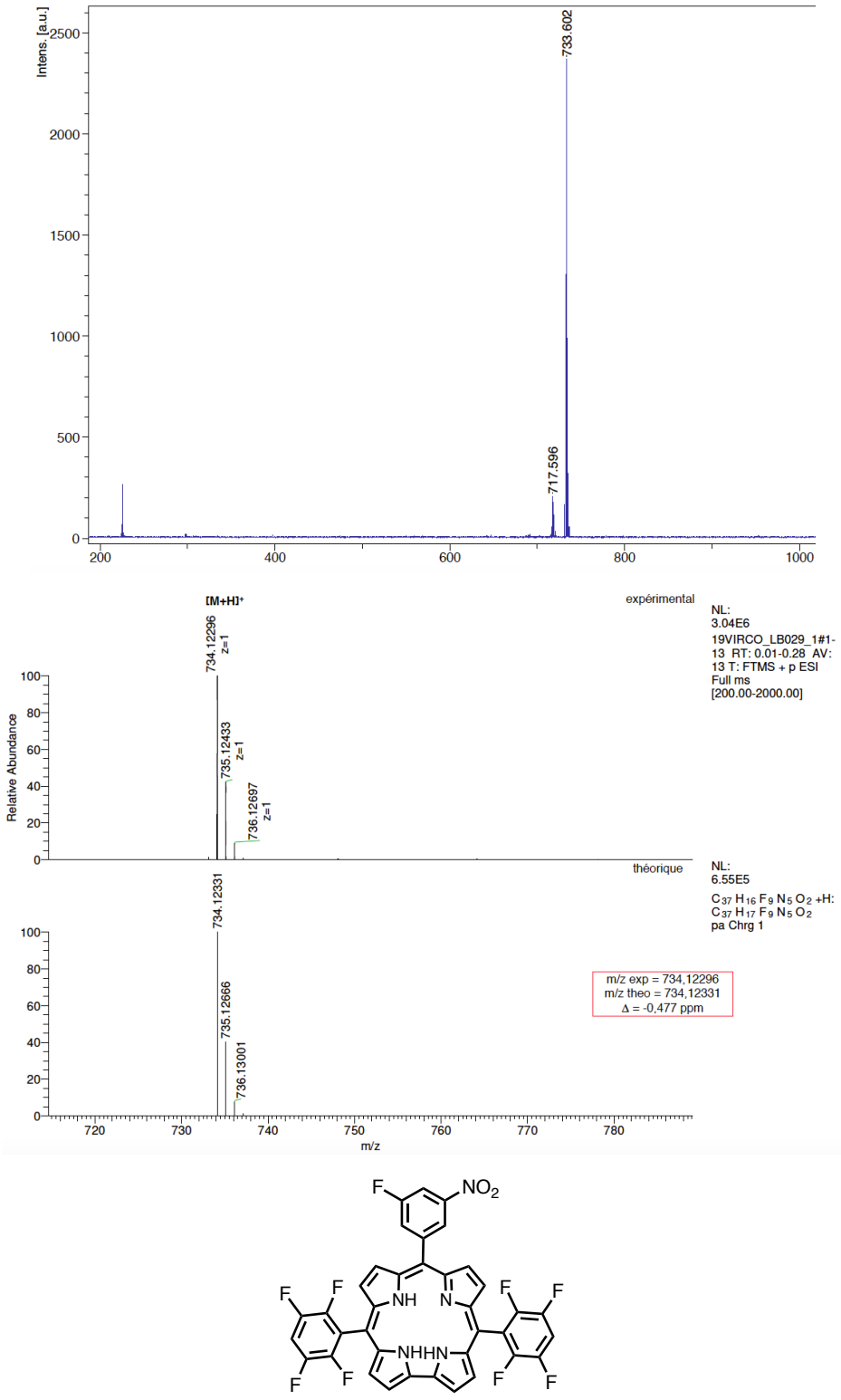


Figure S73: HPLC chromatogram of 5,15-bis(3'-fluoro-5'-nitrophenyl)-10-(2',3',5',6'-tetrafluorophenyl)corrole **25**.



Chemical Formula: $C_{37}H_{16}F_9N_5O_2$

Exact Mass: 733.1160

Molecular Weight: 733.5536

Figure S74: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(3'-fluoro-5'-nitrophenyl)corrole **26**.

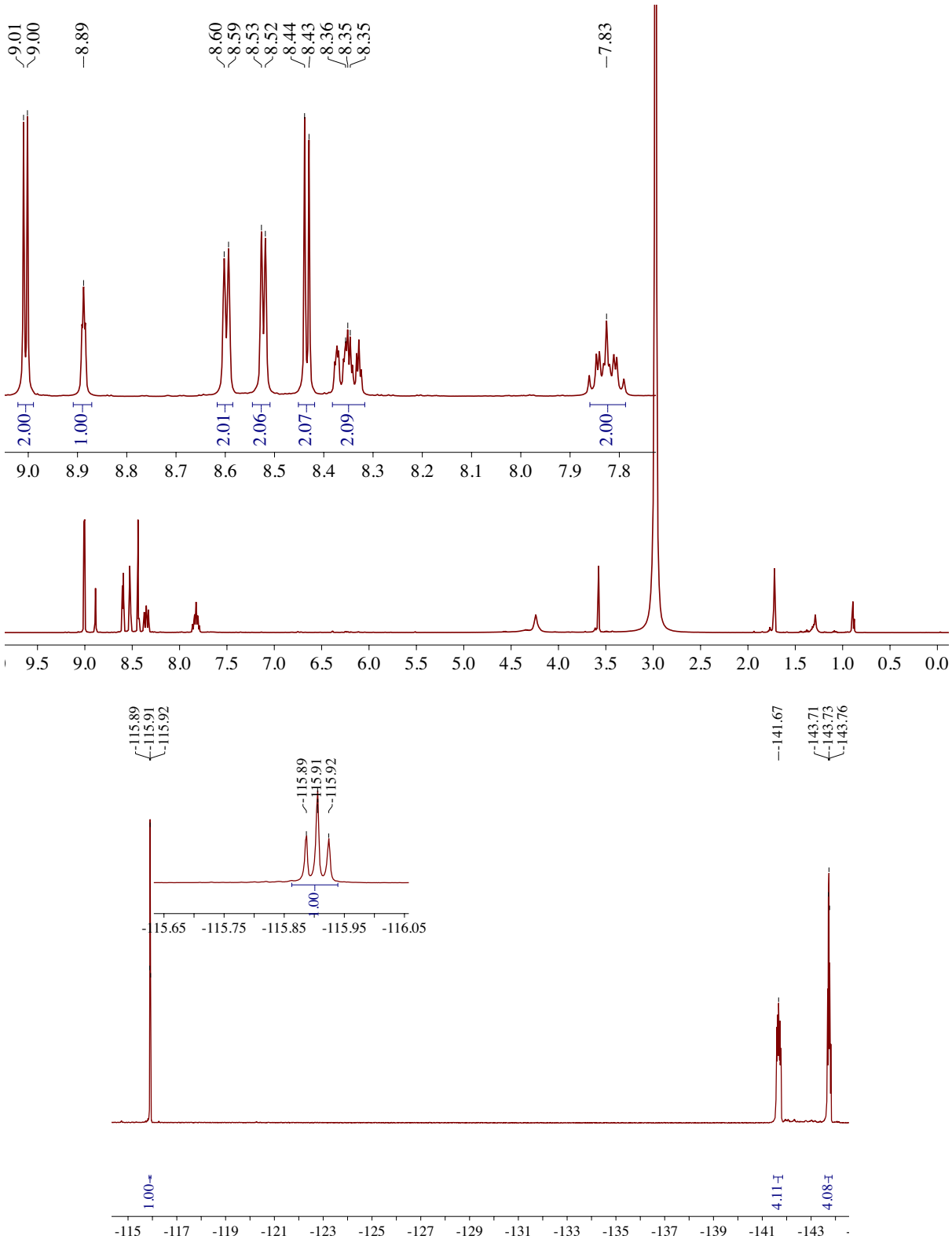


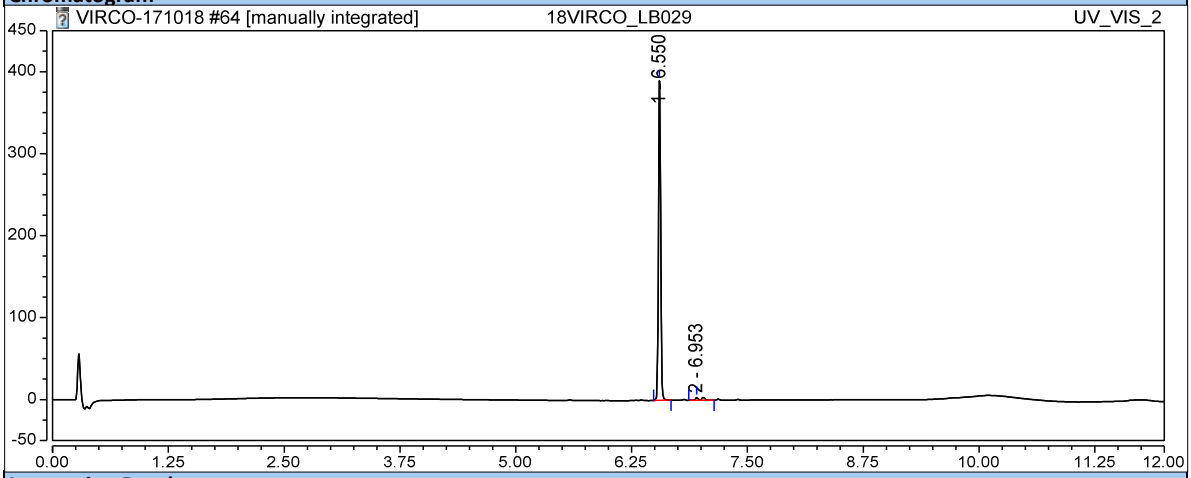
Figure S75: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(3'-fluoro-5'-nitrophenyl)corrole **26** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

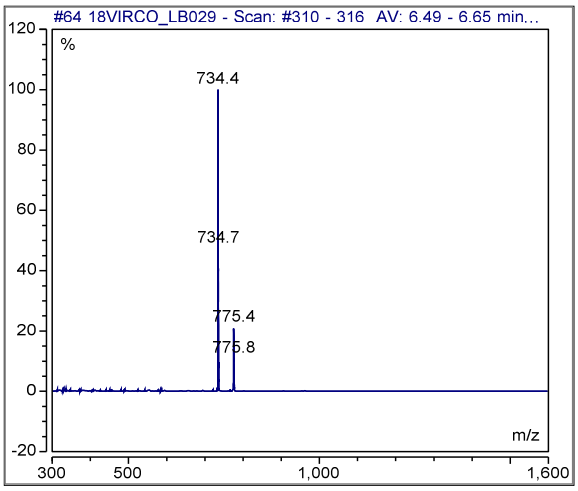
Injection Name:	**18VIRCO_LB029**	*Run Time (min):*	**12.00**
Vial Number:	**GD6**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**18/Apr/19 20:44**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.550	11.022	390.011	97.69	99.01	n.a.
2		6.953	0.260	3.895	2.31	0.99	n.a.
Total:			**11.283**	**393.906**	**100.00**	**100.00**	



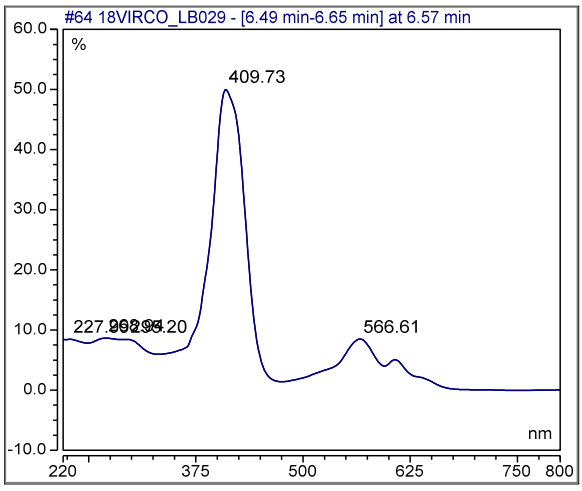
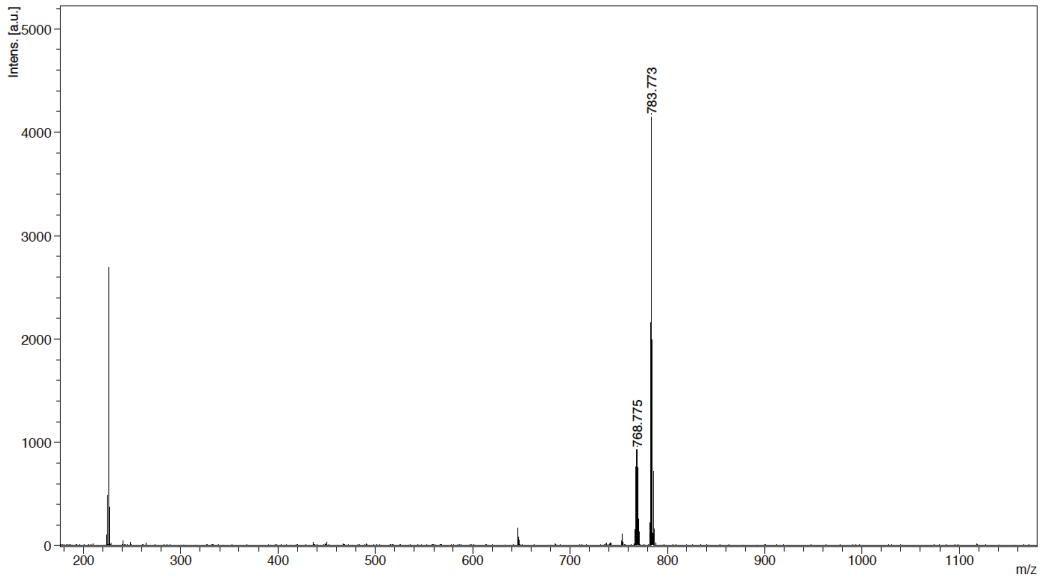
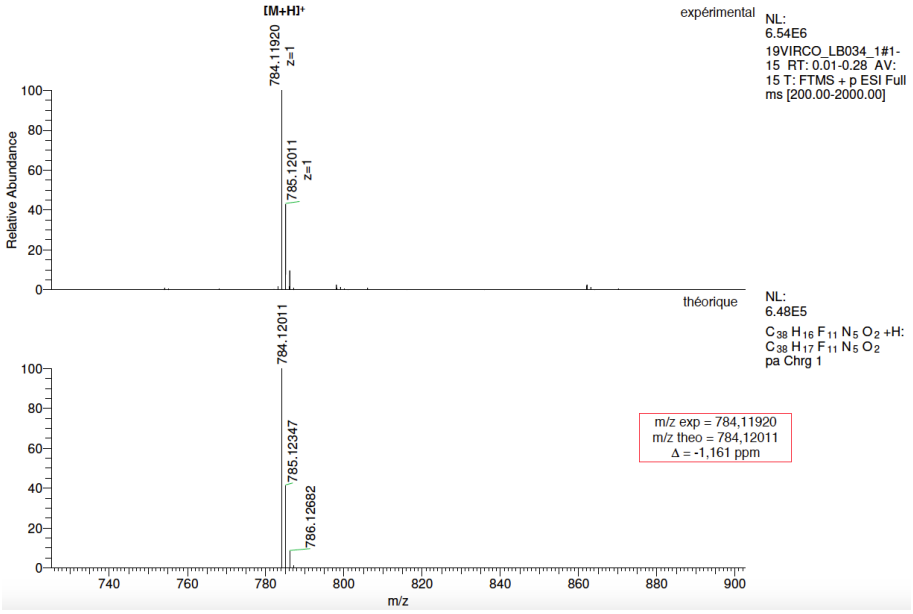
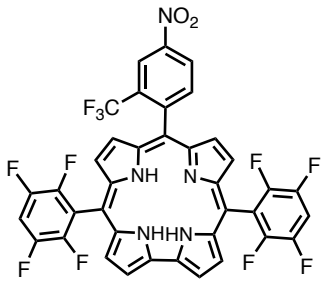


Figure S76: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(3'-fluoro-5'-nitrophenyl)corrole **26**.







Chemical Formula: $C_{38}H_{16}F_{11}N_5O_2$
Exact Mass: 783.1128
Molecular Weight: 783.5614

Figure S77: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(4'-nitro-2'-trifluoromethylphenyl)corrole **27**.

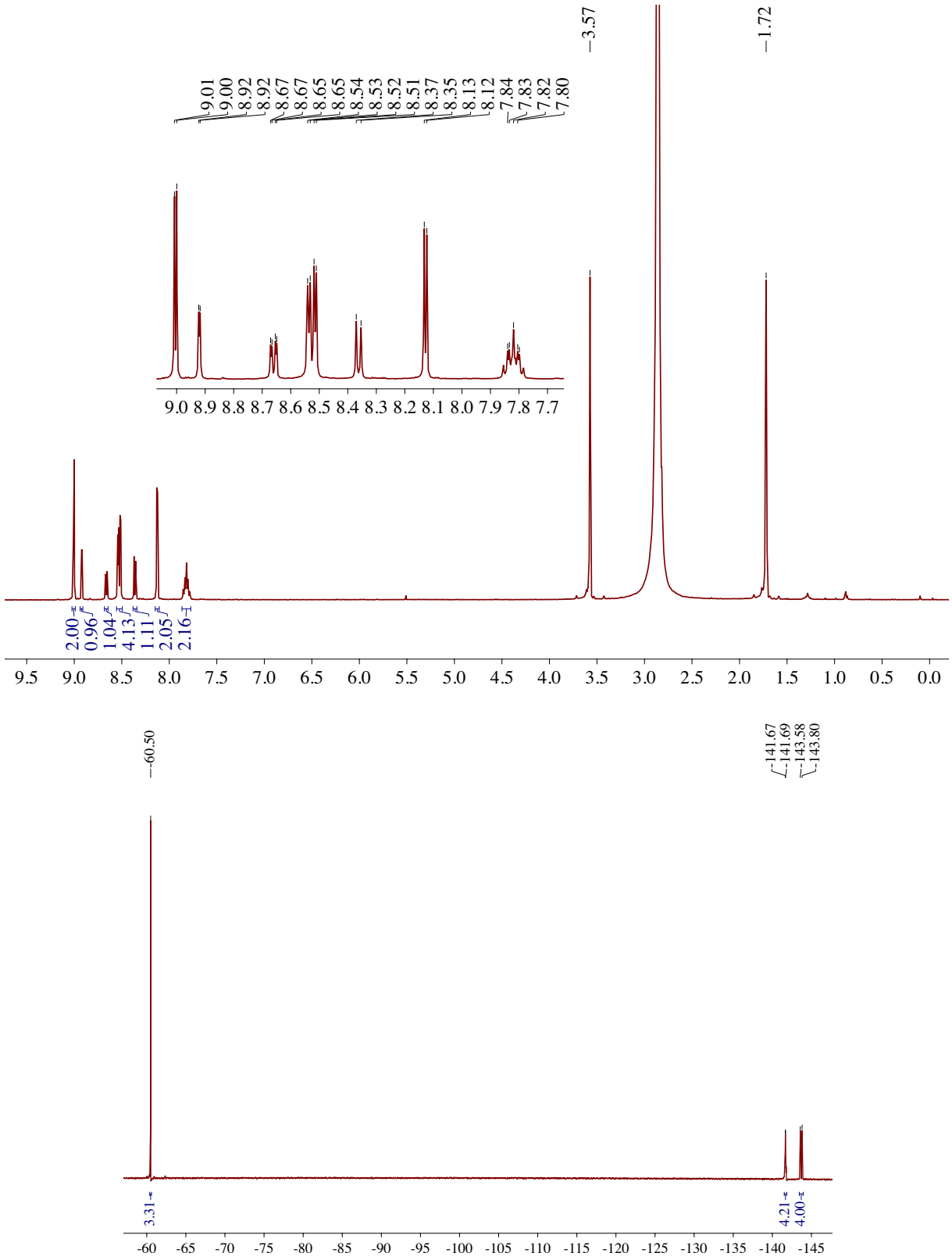


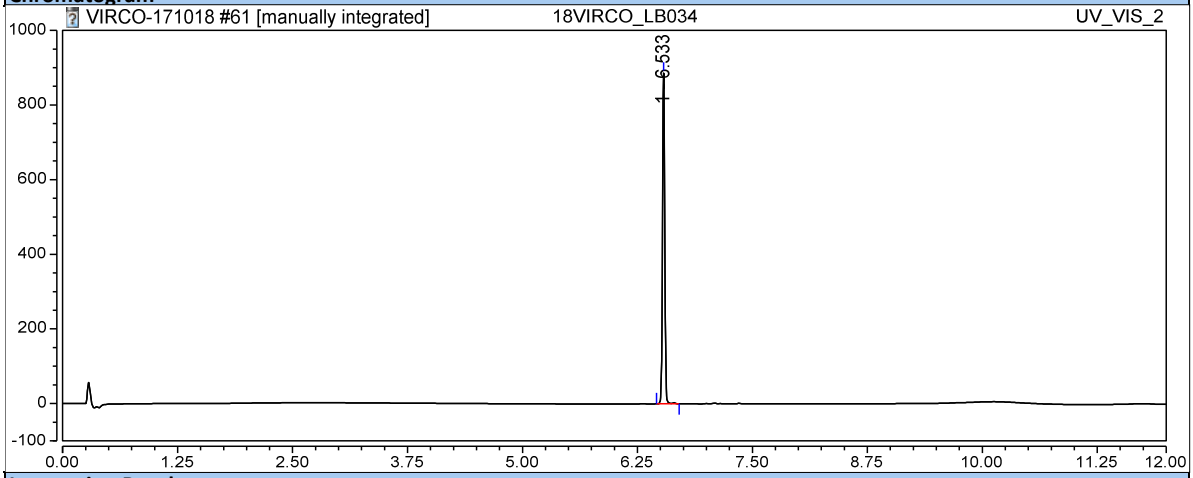
Figure S78: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(4'-nitro-2'-trifluoromethylphenyl)corrole **27** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

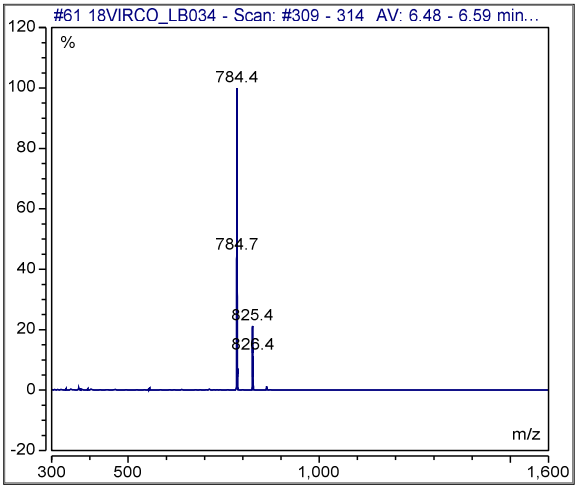
Injection Name:	**18VIRCO_LB034**	*Run Time (min):*	**12.00**
Vial Number:	**BB2**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**18/Apr/19 17:48**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.533	24.935	886.426	100.00	100.00	n.a.
Total:			**24.935**	**886.426**	**100.00**	**100.00**	



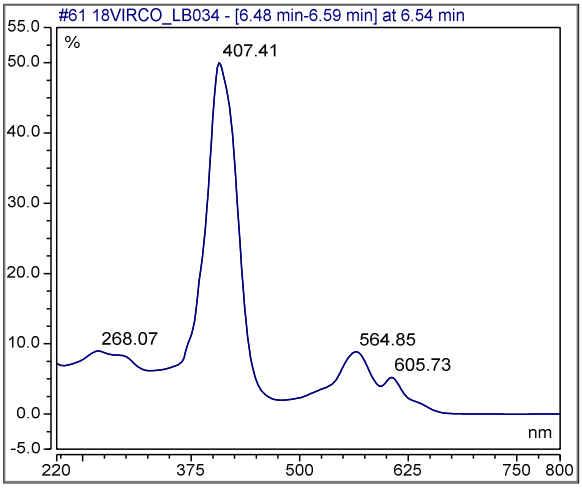
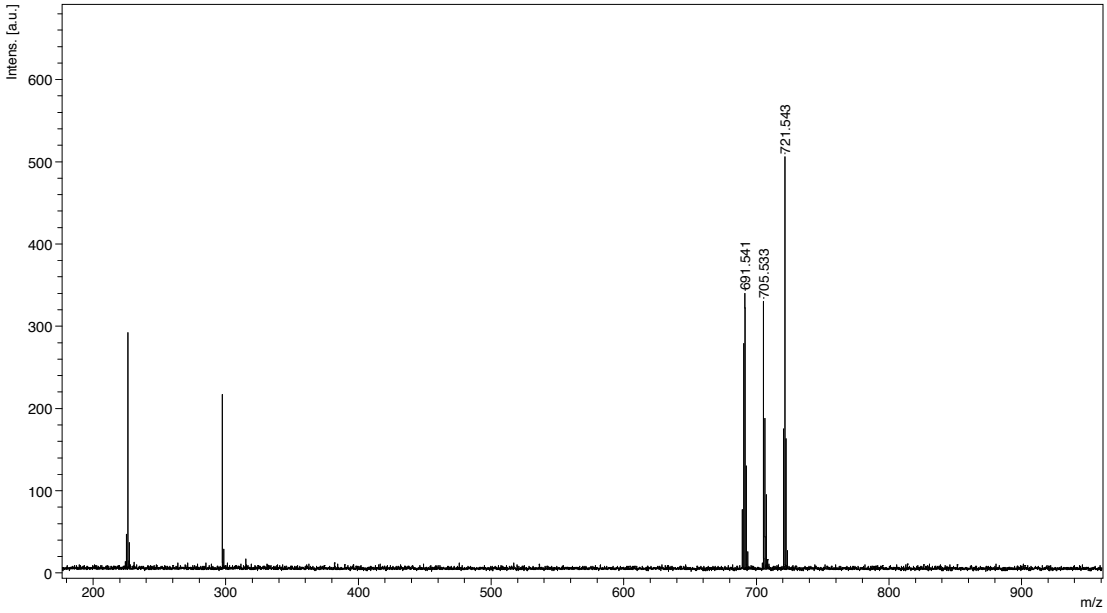
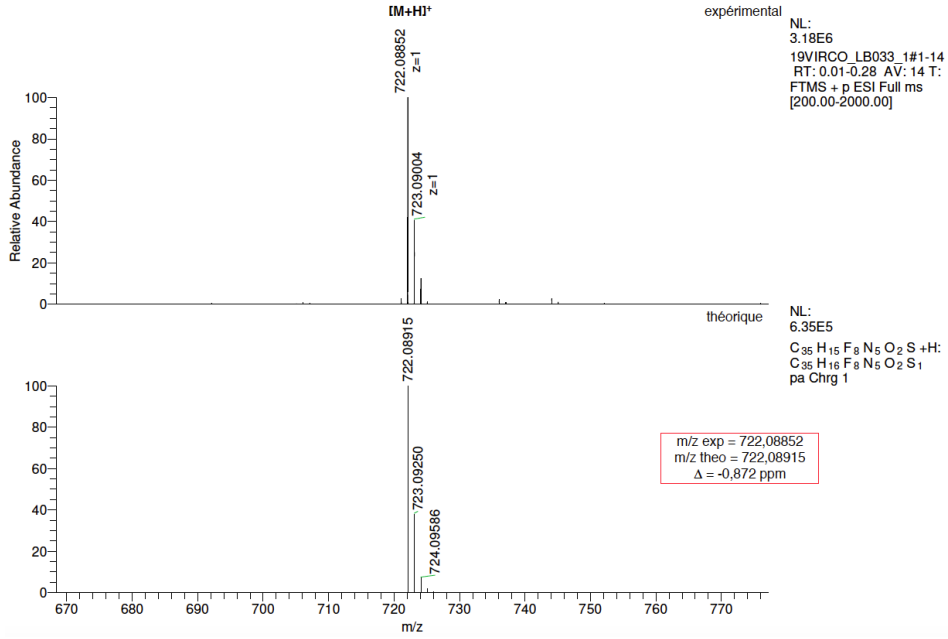
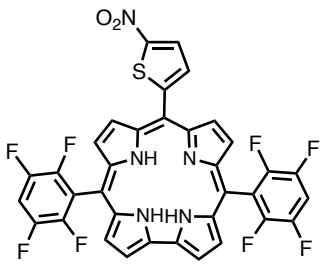


Figure S79: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(4'-nitro-2'-trifluoromethylphenyl)corrole **27**.







Chemical Formula: $C_{35}H_{15}F_8N_5O_2S$
Exact Mass: 721.0819
Molecular Weight: 721.5852

Figure S80: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(5'-nitrothien-2'-yl)corrole **28**.

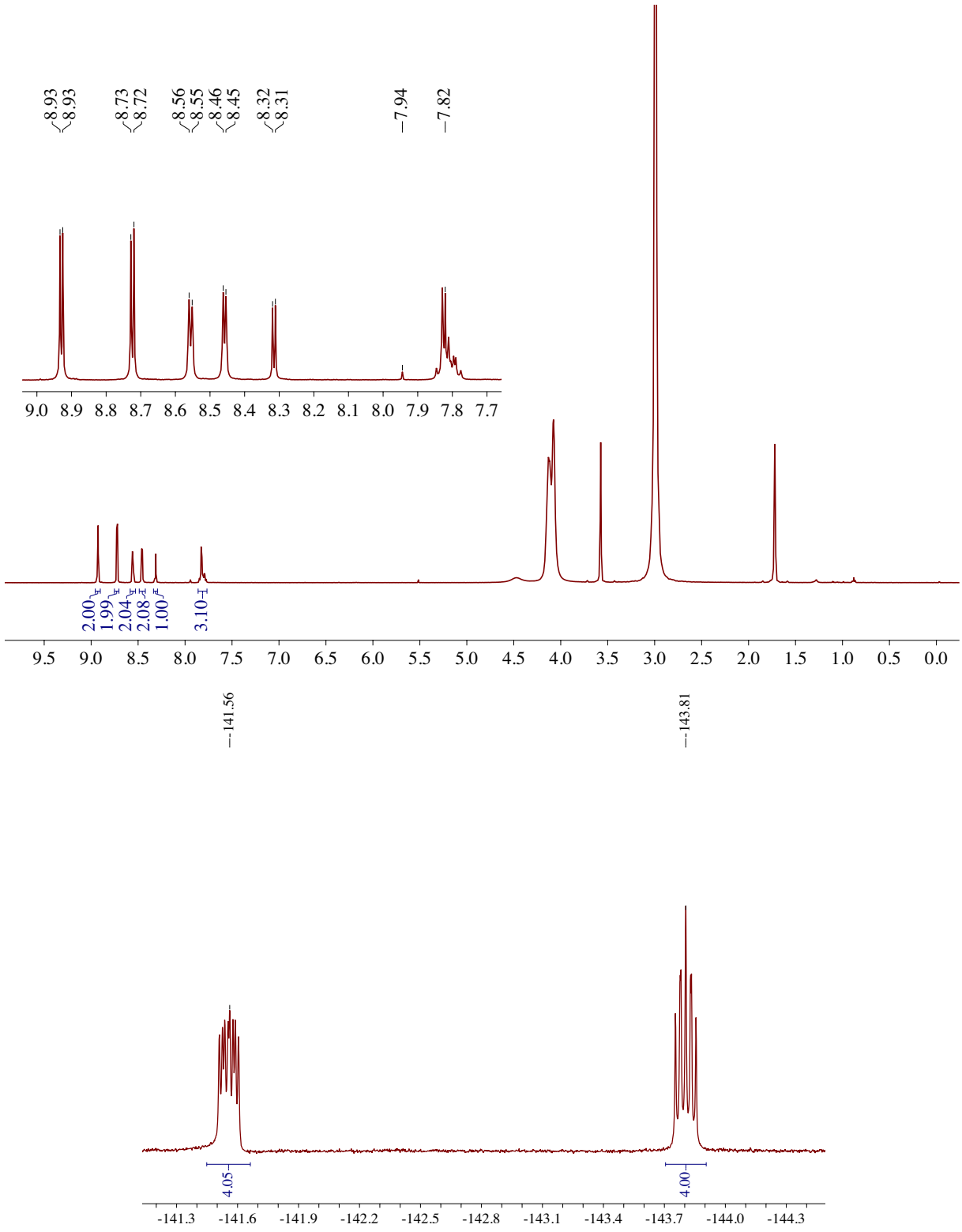


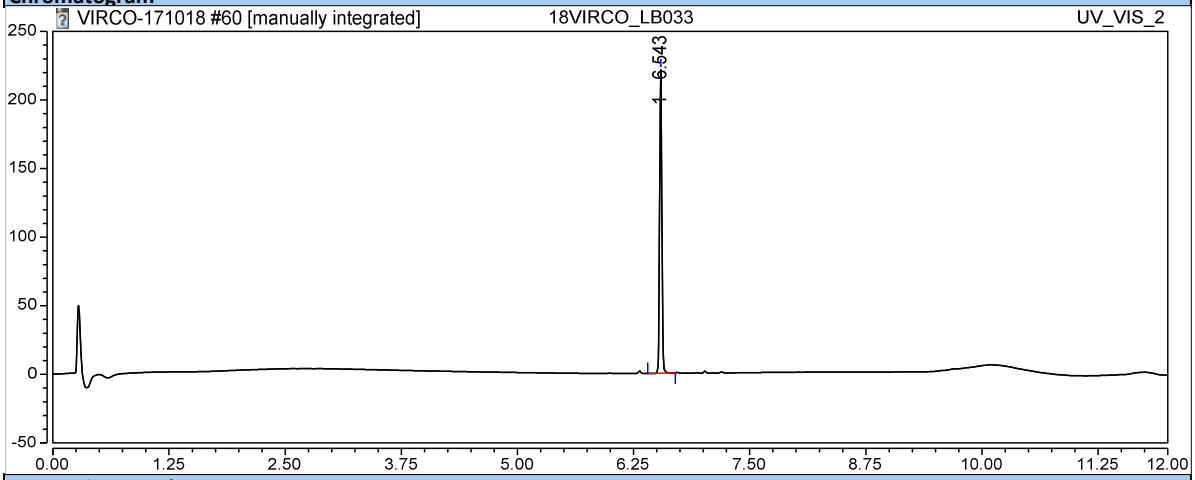
Figure S81: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(5'-nitrothien-2'-yl)corrole **28** in THF-d_8 + one drop of hydrazine hydrate 64%.

Chromatogram and Results

Injection Details

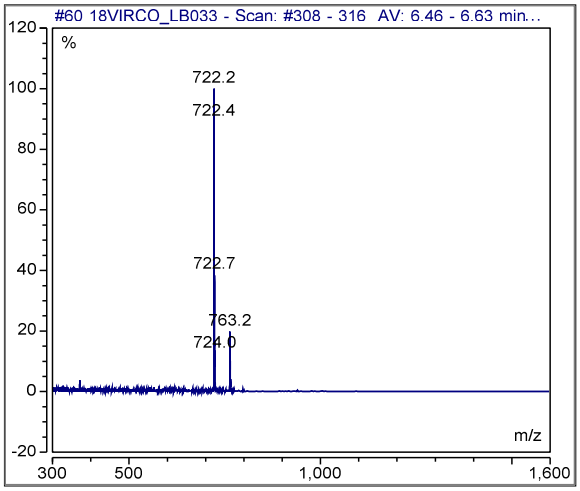
Injection Name:	**18VIRCO_LB033**	*Run Time (min):*	**12.00**
Vial Number:	**BB1**	*Injection Volume:*	**10.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_2**
Calibration Level:		*Wavelength:*	**400.0**
Instrument Method:	**Corroles-LB-Kinetex**	*Bandwidth:*	**4**
Processing Method:	**no integration**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**18/Apr/19 17:35**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.543	6.201	221.187	100.00	100.00	n.a.
Total:			**6.201**	**221.187**	**100.00**	**100.00**	



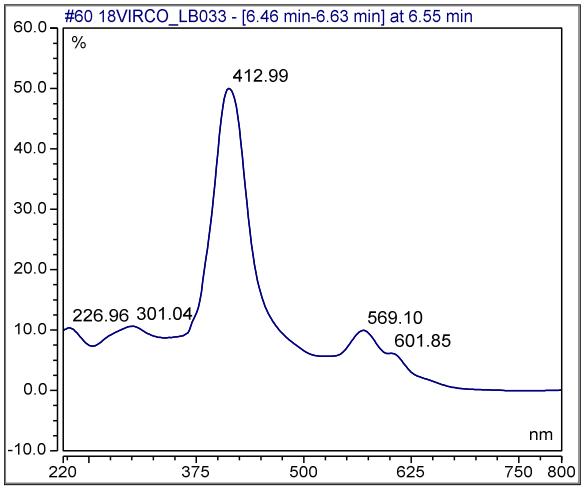
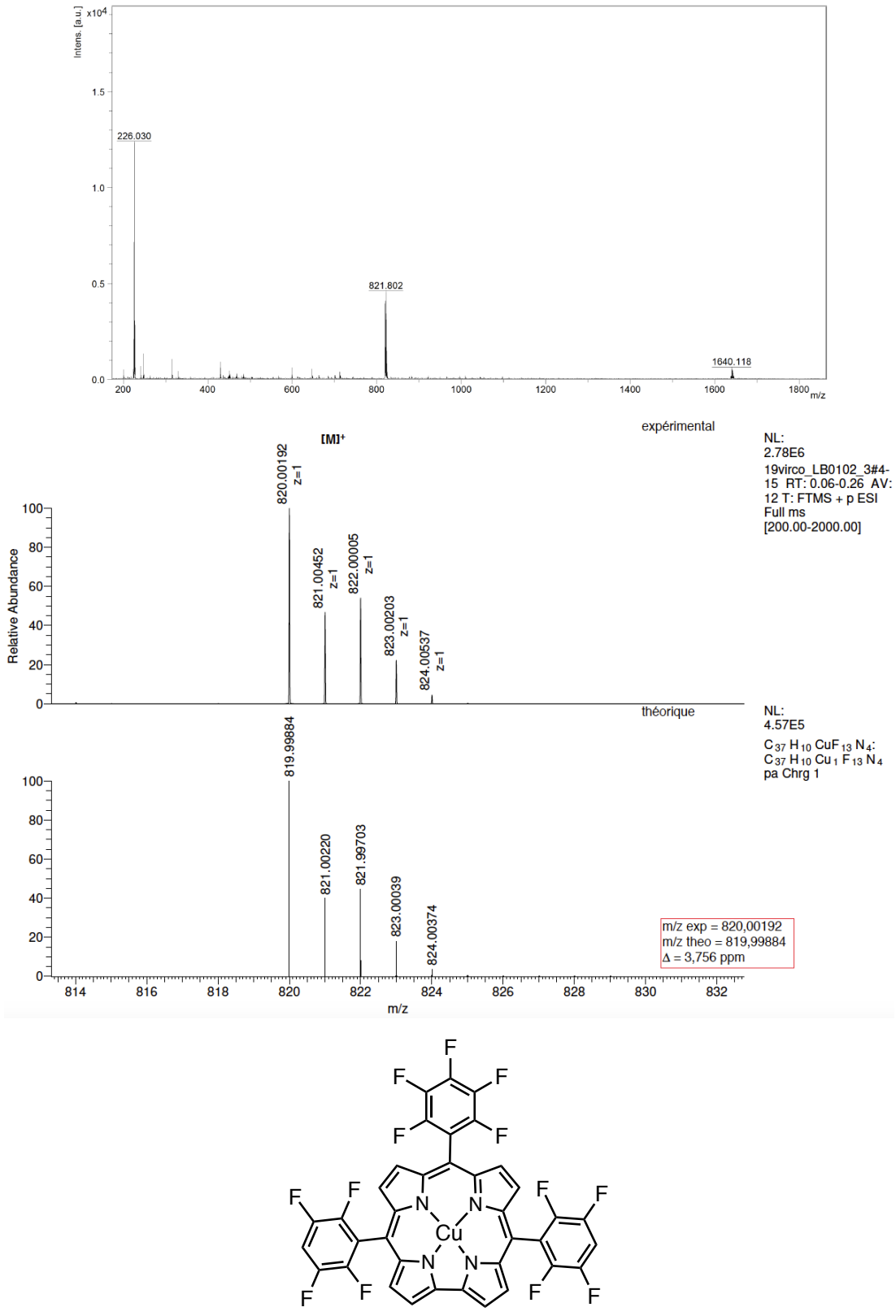


Figure S82: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(5'-nitrothien-2'-yl)corrole **28**.



Chemical Formula: $C_{37}H_{10}CuF_{13}N_4$

Exact Mass: 819.9994

Molecular Weight: 821.0402

Figure S83: MALDI/TOF LRMS and ESI HRMS mass spectra of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pentafluorophenyl)corrole Cu(III) **29**.

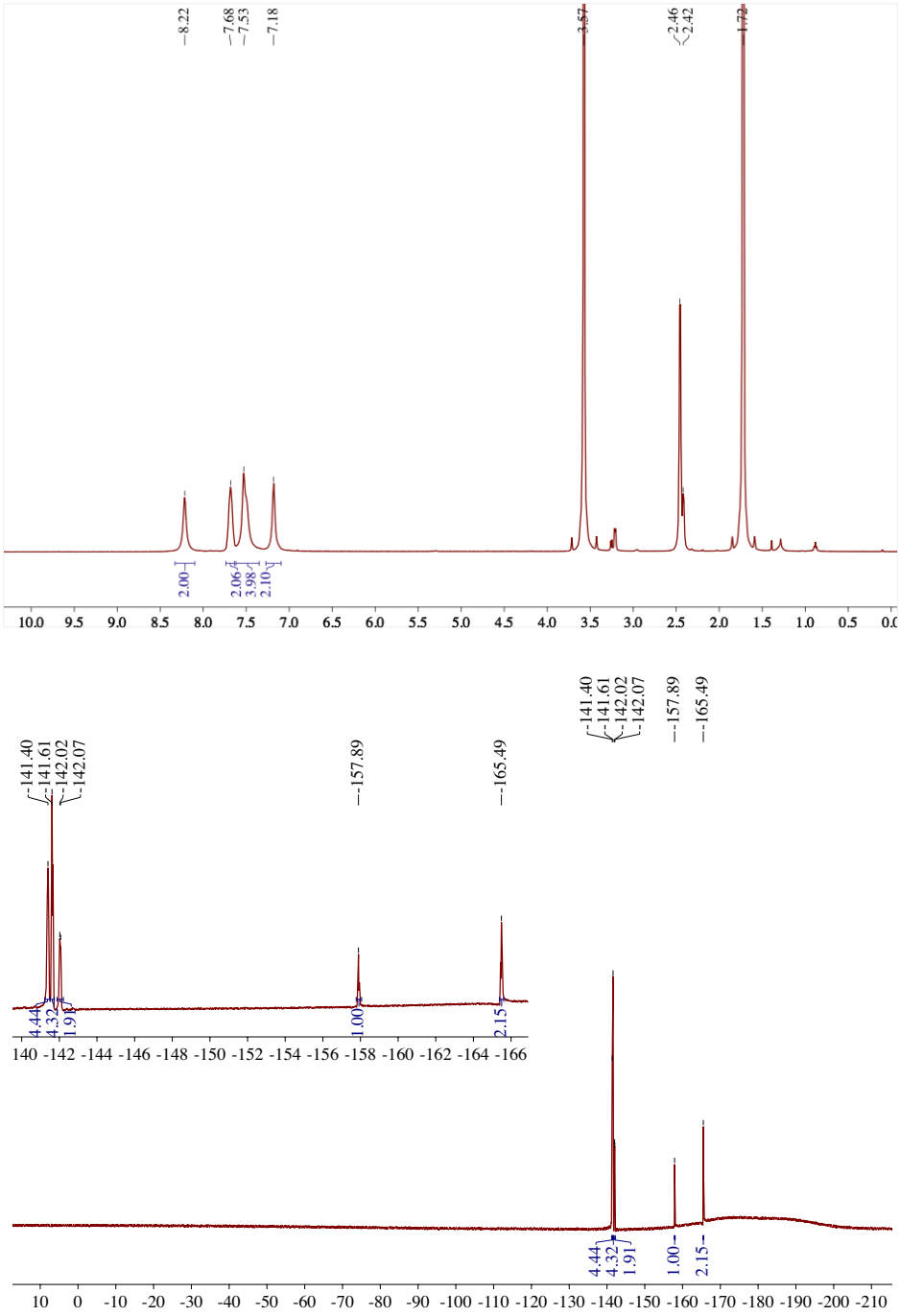


Figure S84: [1]H NMR (top) and [19]F spectra (down) of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pentafluorophenyl)corrole Cu(III) **29** in THF-d_8 + one drop of hydrazine hydrate 64%.

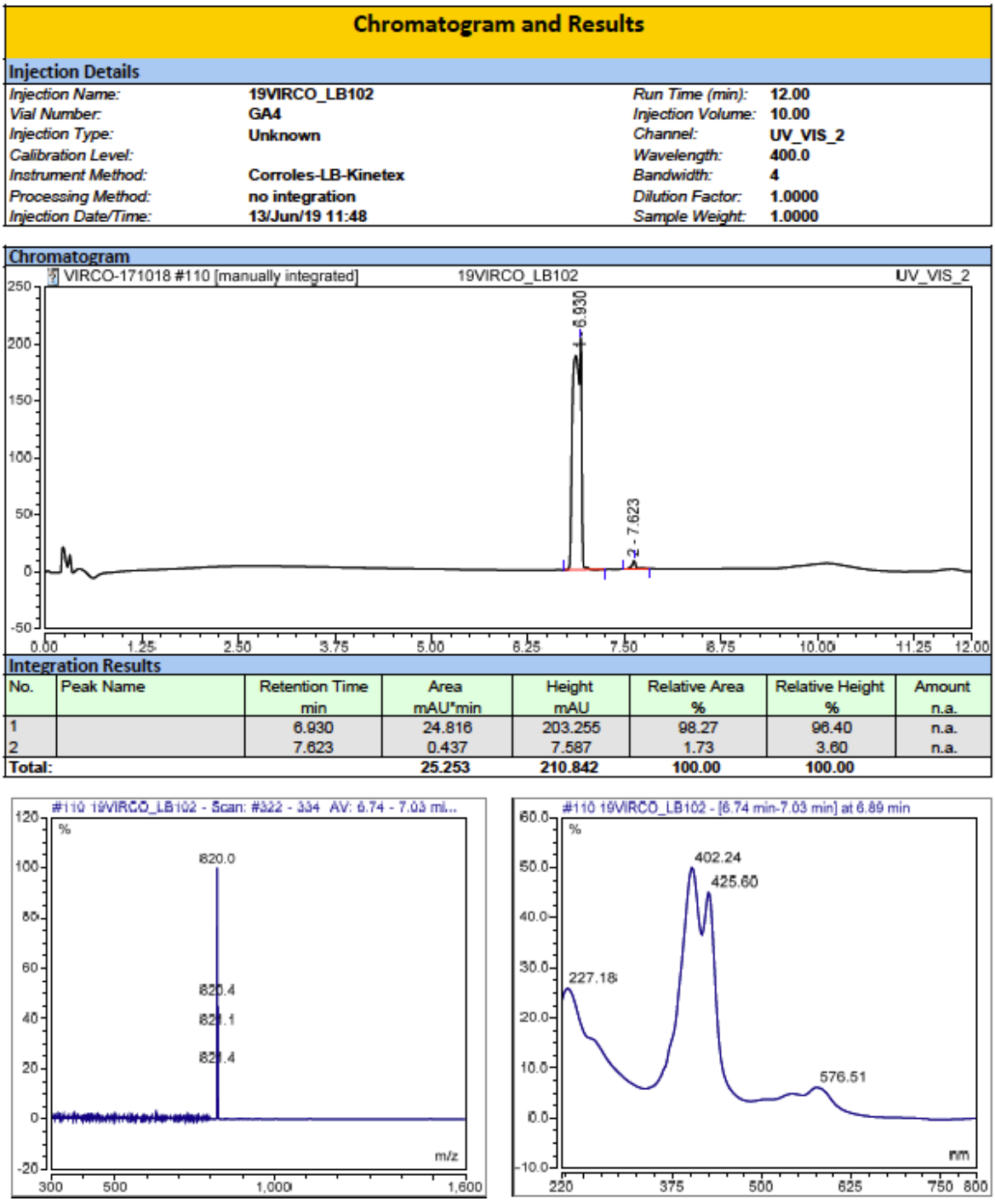
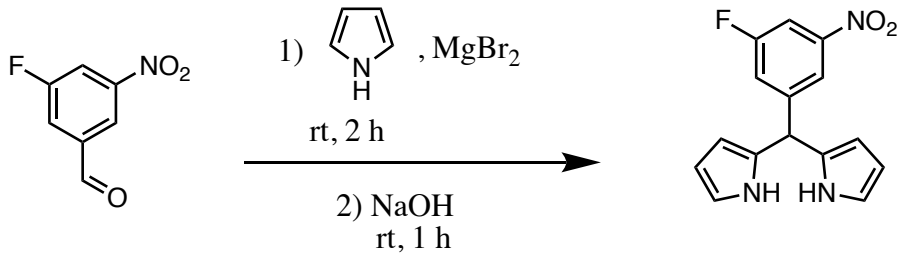


Figure S85: HPLC chromatogram of 5,15-bis(2',3',5',6'-tetrafluorophenyl)-10-(pentafluorophenyl)corrole Cu(III) **29**.

Synthesis of 5-(3'-Fluoro-5'-nitrophenyl)-dipyrromethane

3-Fluoro-5-nitrobenzaldehyde (1.53 g, 9.05 mmol), purchased from Fluorochem, was added to pyrrole (67.8 mL, 904.74 mmol) in a round-bottom flask. Magnesium bromide (833.1 mg, 4.53 mmol) was introduced afterwards, then the reaction was left stirring in the dark at room temperature for 2 h. This solution was stirred one more hour after addition of sodium hydroxide in powder (1.81 g, 45.25 mmol). The mixture was filtrated over a Dicalite® plug and evaporated to dryness. The oily residue was purified with a SiO_2 plug (heptane/ethyl acetate 8:2) and subsequent washings with heptane and pentane to afford the dipyrromethane as a yellow solid with 71.0% yield (1.83 g).



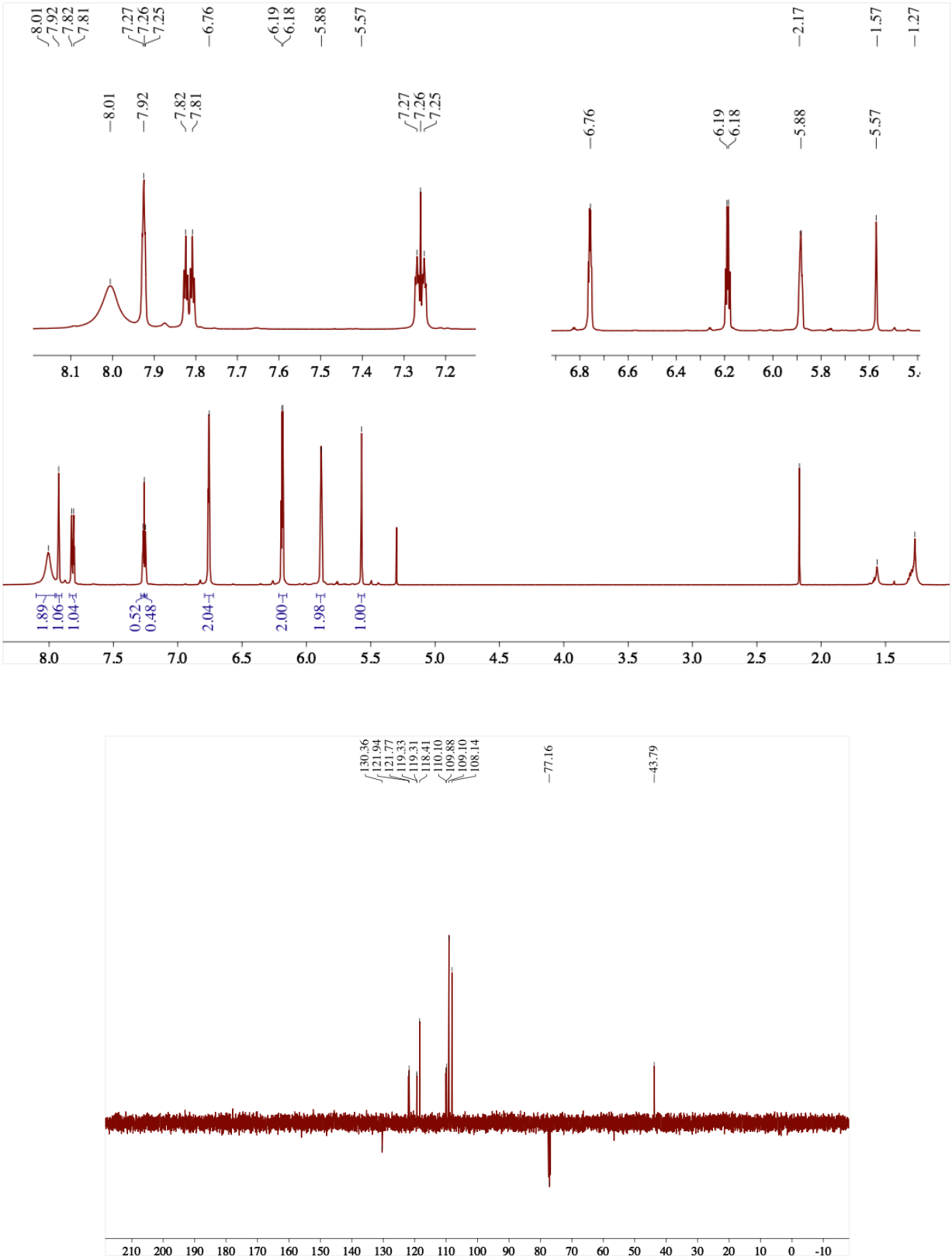
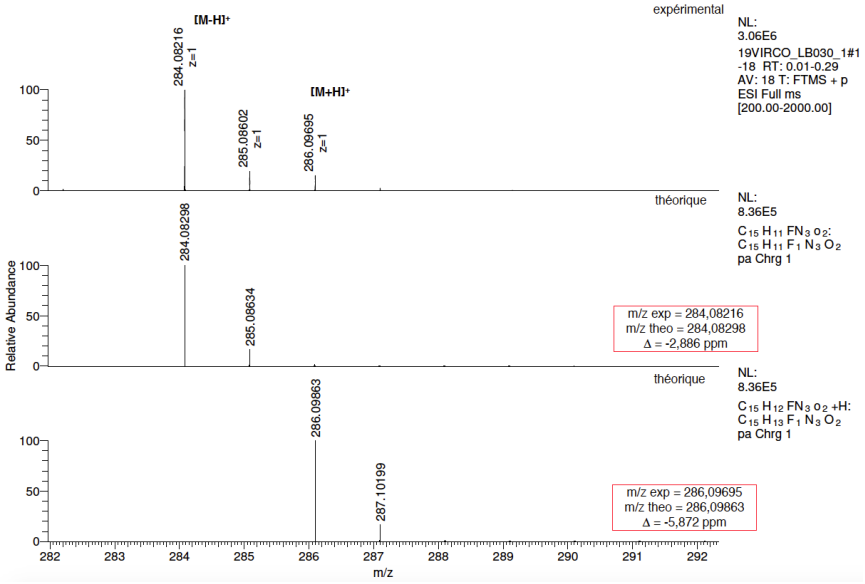


Figure S86: ^{1}H (500 MHz, top) and ^{13}C (125 MHz, above) NMR spectra ($CDCl_3$) of 5-(3'-fluoro-5'-nitrophenyl)-dipyrromethane.



Chemical Formula: $C_{15}H_{12}FN_3O_2$
Exact Mass: 285.09
Molecular Weight: 285.28

Figure S87: ESI HRMS mass spectrum of 5-(3'-fluoro-5'-nitrophenyl)-dipyrromethane.

A

	1	2	3	4	5	6	7	8	9	10	11	12		
A	DMSO	DMSO	DMSO	DMSO	DMSO	DMSO	DMSO	DMSO	DMSO	DMSO	DMSO	DMSO		
B	DMSO	DMSO	DMSO	10	5	2,5	1,25	0,625	0,3125	0,156	0,078	0,039	GCV	f=1
C	DMSO	0,078	0,039	DMSO	DMSO	10	5	2,5	1,25	0,625	0,3125	0,156		f=0,8
D	DMSO	0,3125	0,156	0,078	0,039	DMSO	DMSO	10	5	2,5	1,25	0,625		f=0,65
E	DMSO	1,25	0,625	0,3125	0,156	0,078	0,039	DMSO	DMSO	10	5	2,5		f=0,5
F	DMSO	5	2,5	1,25	0,625	0,3125	0,156	0,078	0,039	DMSO	DMSO	10		f=0,35
G	DMSO	DMSO	10	5	2,5	1,25	0,625	0,3125	0,156	0,078	0,039	DMSO		f=0,2
H	DMSO	10	5	2,5	1,25	0,625	0,3125	0,156	0,078	0,039	DMSO	DMSO	LB003	f=0

	10		5		2,5		1,25		0,625		0,3125		0,156		0,078		0,039	
f	GCV	LB003	GCV	LB003	GCV	LB003	GCV	LB003	GCV	LB003	GCV	LB003	GCV	LB003	GCV	LB003	GCV	LB003
1	25	0	12,5	0	6,25	0	3,125	0	1,56	0	0,78	0	0,39	0	0,19	0	0,097	0
0,8	20	2,38	10	1,19	5	0,60	2,50	0,30	1,25	0,15	0,63	0,07	0,31	0,04	0,16	0,02	0,08	0,01
0,65	16,25	4,165	8,125	2,0825	4,0625	1,04	2,03	0,52	1,02	0,26	0,51	0,13	0,25	0,06	0,13	0,03	0,06	0,02
0,5	12,5	5,95	6,25	2,975	3,125	1,49	1,56	0,74	0,78	0,37	0,39	0,19	0,19	0,09	0,10	0,05	0,05	0,02
0,35	8,75	7,735	4,375	3,8675	2,1875	1,93	1,09	0,97	0,55	0,48	0,27	0,24	0,14	0,12	0,07	0,06	0,03	0,03
0,2	5	9,52	2,5	4,76	1,25	2,38	0,63	1,19	0,31	0,60	0,16	0,30	0,08	0,15	0,04	0,07	0,02	0,04
0	0	11,9	0	5,95	0	2,98	0,00	1,49	0,00	0,74	0,00	0,37	0,00	0,19	0,00	0,09	0,00	0,05

Figure S88: plate layout for combinatorial studies of compound **17** and Ganciclovir.

Compound 15

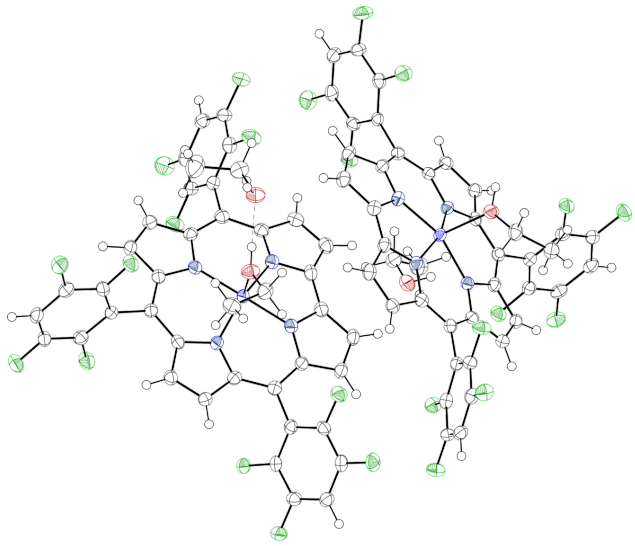
Report created with **ReportPlus**

Submitted by: **Léo Bucher**

Solved by: **Yoann Rousselin**

Sample ID: **20181008LB055**

Crystal Data and Experimental



Experimental. Single clear dark violet prism-shaped crystals of **15** were recrystallized from a mixture of ethanol and ethyl acetate by slow evaporation. A suitable crystal 0.50 mm x 0.09 mm x 0.08 mm was selected and mounted on a MITIGEN holder oil on an Bruker D8 Venture (Cu) diffractometer. The crystal was kept at a steady T = 100(1) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using the Intrinsic Phasing solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2018/3 of **ShelXL** (Sheldrick, 2015) using Least Squares minimization.

Crystal Data. $C_{41}H_{23}F_{12}MnN_4O_2$, M_r = 886.57, triclinic, P-1 (No. 2), a = 7.5565(3) Å, b = 17.8342(7) Å, c = 26.0523(10) Å, α = 95.3050(16)°, β = 90.3264(16)°, γ = 97.8043(17)°, V = 3462.9(2) Å^3, T = 100(1) K, Z = 4, Z' = 2, μ(CuK$_\alpha$) = 4.109, 21719 reflections measured, 21719 unique (R_{int} = .) which were used in all calculations. The final wR_2 was 0.1367 (all data) and R_1 was 0.0523 (I > 2(I)).

Compound	**15**
CCDC	**1910514**
Formula	$C_{41}H_{23}F_{12}MnN_4O_2$
$D_{calc.}$/ g cm^{-3}	1.701
μ/mm^{-1}	4.109
Formula Weight	886.57
Colour	clear dark violet
Shape	prism
Size/mm^3	0.50x0.09x0.08
T/K	100(1)
Crystal System	Triclinic
Space Group	P-1
a/Å	7.5565(3)
b/Å	17.8342(7)
c/Å	26.0523(10)
α/°	95.3050(16)
β/°	90.3264(16)
γ/°	97.8043(17)
V/Å^3	3462.9(2)
Z	4
Z'	2
Wavelength/Å	1.541840
Radiation type	CuK$_\alpha$
Θ_{min}/°	2.900
Θ_{max}/°	66.680
Measured Refl.	21719
Independent Refl.	21719
Reflections with I > 2(I)	18498
R_{int}	.
Parameters	1090
Restraints	0
Largest Peak	0.489
Deepest Hole	-0.598
GooF	1.028
wR_2 (all data)	0.1367
wR_2	0.1295
R_1 (all data)	0.0629
R_1	0.0523

Structure Quality Indicators

Reflections:	d min (Cu) 0.84	I/σ 18.5	Rint Merged!	complete 99%
Refinement:	Shift -0.001	Max Peak 0.5	Min Peak -0.6	GooF 1.028

A clear dark violet prism-shaped crystal with dimensions 0.50 mm x 0.09 mm x 0.08 mm was mounted on a MITIGEN holder oil. Data were collected using an Bruker D8 Venture (Cu) diffractometer equipped with an Oxford Cryosystems low-temperature device operating at T = 100(1) K. Data were measured using ϕ and ω scans using CuK_α radiation. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) The maximum resolution that was achieved was Θ = 66.680° (0.84 Å). The diffraction pattern was indexed. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) and the unit cell was refined using **SAINT** (Bruker, V8.38A, after 2013) on 9726 reflections, 45% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.38A, after 2013). The final completeness is 97.40 % out to 66.680° in Θ. A multi-scan absorption correction was performed using **TWINABS-2012/1** (Bruker, 2012) was used for absorption correction. Final HKLF 4 output contains 46918 reflections, R_{int} = 0.0568 (35482 with I > 3sig(I), R_{int} = 0.0531). The absorption coefficient μ of this material is 4.109 mm^{-1} at this wavelength (λ = 1.542Å) and the minimum and maximum transmissions are 0.400 and 0.580. The structure was solved and the space group P-1 (# 2) determined by the **ShelXT** (Sheldrick, 2015) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model. The value of Z' is 2. This means that there are two independent molecules in the asymmetric unit. Refined as a 2-component twin. Several crystals examined proved to have multiple domains. The final data crystal, while still a multiple, could be described having primarily two domains and was treated as such. Orientation matrices for the two domains were determined using the program **CELL_NOW** (Bruker, 2008) and the data were processed further using **TWINABS** (Bruker, 2008). HKLF 5 was employed, BASF specifies the fractional volume contributions of the various twin components. The crystal was refined as a non-merohedral twin with a minor twin component of 0.288(1).

Table 1: Bond Lengths in Å for **15**.

Atom	Atom	Length/Å
Mn1A	O1A	2.144(3)
Mn1A	N1A	1.908(3)
Mn1A	N3A	1.930(3)
Mn1A	N2A	1.936(3)
Mn1A	N4A	1.915(3)
Mn1	O1	2.145(3)
Mn1	N3	1.931(3)
Mn1	N4	1.907(3)
Mn1	N2	1.934(3)
Mn1	N1	1.918(3)
F9A	C27A	1.349(4)
F5	C33	1.347(4)
F12	C31	1.350(4)
F8A	C37A	1.346(4)
F9	C27	1.345(4)
F1A	C21A	1.349(4)
F10	C28	1.353(4)
F4A	C25A	1.346(4)
F6A	C34A	1.348(4)
F12A	C31A	1.350(4)
F2	C22	1.351(4)

Atom	Atom	Length/Å
F2A	C22A	1.342(4)
F6	C34	1.354(4)
F7A	C36A	1.350(4)
F1	C21	1.347(4)
F11A	C30A	1.349(4)
F4	C25	1.352(4)
F8	C37	1.352(4)
F5A	C33A	1.351(4)
F3	C24	1.357(4)
F3A	C24A	1.353(4)
F7	C36	1.350(4)
F11	C30	1.347(4)
F10A	C28A	1.349(4)
O1	C39	1.444(5)
O1A	C39A	1.447(4)
O2A	C40A	1.435(5)
O2	C40	1.433(5)
N1A	C17A	1.374(5)
N1A	C1A	1.361(5)
N3A	C11A	1.393(4)
N3A	C8A	1.381(4)

Atom	Atom	Length/Å
N3	C11	1.395(4)
N3	C8	1.378(5)
N4	C16	1.375(5)
N4	C13	1.364(5)
N2A	C3A	1.388(4)
N2A	C6A	1.388(5)
N2	C3	1.388(5)
N2	C6	1.379(5)
N1	C1	1.363(5)
N1	C17	1.380(5)
N4A	C13A	1.367(5)
N4A	C16A	1.373(5)
C3	C2	1.403(5)
C3	C4	1.429(5)
C21A	C20A	1.383(5)
C21A	C22A	1.387(5)
C34A	C33A	1.387(5)
C34A	C35A	1.377(6)
C13A	C12A	1.406(5)
C13A	C14A	1.427(5)
C31A	C26A	1.387(5)
C31A	C30A	1.378(5)
C32	C7	1.492(5)
C32	C33	1.394(5)
C32	C37	1.379(5)
C36A	C37A	1.375(5)
C36A	C35A	1.373(6)
C37A	C32A	1.393(5)
C4A	C5A	1.357(5)
C4A	C3A	1.431(5)
C27A	C26A	1.392(5)
C27A	C28A	1.372(5)
C7	C6	1.413(5)
C7	C8	1.412(5)
C26A	C12A	1.489(5)
C33	C34	1.380(5)
C6	C5	1.432(5)
C24A	C25A	1.380(5)
C24A	C23A	1.371(5)
C11	C12	1.409(5)
C11	C10	1.431(5)
C23	C22	1.380(6)
C23	C24	1.372(6)
C8	C9	1.439(5)
C32A	C33A	1.383(5)
C32A	C7A	1.493(5)
C5A	C6A	1.431(5)
C17A	C16A	1.407(5)
C17A	C18A	1.418(5)
C30A	C29A	1.376(6)
C16A	C15A	1.422(5)
C29	C28	1.373(5)
C29	C30	1.384(5)
C28A	C29A	1.378(6)
C27	C28	1.381(5)
C27	C26	1.394(5)
C37	C36	1.379(5)
C9	C10	1.367(5)
C3A	C2A	1.408(5)
C20	C21	1.387(5)
C20	C2	1.499(5)
C20	C25	1.394(5)
C25A	C20A	1.389(5)
C5	C4	1.366(5)
C26	C12	1.488(5)
C26	C31	1.389(5)
C16	C17	1.408(5)
C16	C15	1.418(5)
C18A	C19A	1.377(5)
C1A	C19A	1.430(5)
C1A	C2A	1.404(5)
C21	C22	1.378(5)
C1	C2	1.410(5)
C1	C19	1.426(5)
C11A	C12A	1.410(5)
C11A	C10A	1.421(5)
C12	C13	1.411(5)
C36	C35	1.378(6)
C13	C14	1.430(5)
C7A	C8A	1.418(5)
C7A	C6A	1.407(5)
C20A	C2A	1.491(5)
C34	C35	1.366(6)
C31	C30	1.374(5)
C17	C18	1.421(5)
C15A	C14A	1.376(5)
C22A	C23A	1.379(5)
C24	C25	1.376(5)
C8A	C9A	1.430(5)
C19	C18	1.370(5)
C39A	C38A	1.497(5)
C10A	C9A	1.370(5)
C39	C38	1.502(6)
C41	C40	1.499(6)
C40A	C41A	1.497(6)
C14	C15	1.375(5)

Table 2: Bond Angles in ° for **15**.

Atom	Atom	Atom	Angle/°
N1A	Mn1A	O1A	99.19(12)
N1A	Mn1A	N3A	161.57(13)
N1A	Mn1A	N2A	89.27(12)
N1A	Mn1A	N4A	80.44(12)
N3A	Mn1A	O1A	98.13(11)
N3A	Mn1A	N2A	96.03(12)
N2A	Mn1A	O1A	93.16(11)
N4A	Mn1A	O1A	104.51(12)
N4A	Mn1A	N3A	89.17(12)
N4A	Mn1A	N2A	160.71(13)
N3	Mn1	O1	91.82(12)
N3	Mn1	N2	96.45(13)
N4	Mn1	O1	99.78(12)
N4	Mn1	N3	89.30(12)
N4	Mn1	N2	161.95(13)
N4	Mn1	N1	80.75(13)
N2	Mn1	O1	97.13(12)
N1	Mn1	O1	105.69(12)

Atom	Atom	Atom	Angle/°
N1	Mn1	N3	161.04(13)
N1	Mn1	N2	88.67(13)
C39	O1	Mn1	128.2(2)
C39A	O1A	Mn1A	127.0(2)
C17A	N1A	Mn1A	117.1(2)
C1A	N1A	Mn1A	132.8(2)
C1A	N1A	C17A	109.9(3)
C11A	N3A	Mn1A	128.3(2)
C8A	N3A	Mn1A	123.3(2)
C8A	N3A	C11A	108.3(3)
C11	N3	Mn1	127.5(2)
C8	N3	Mn1	122.1(2)
C8	N3	C11	108.5(3)
C16	N4	Mn1	117.0(2)
C13	N4	Mn1	133.1(2)
C13	N4	C16	109.6(3)
C3A	N2A	Mn1A	127.1(2)
C3A	N2A	C6A	108.4(3)
C6A	N2A	Mn1A	122.5(2)
C3	N2	Mn1	128.8(2)
C6	N2	Mn1	122.4(2)
C6	N2	C3	108.7(3)
C1	N1	Mn1	133.6(3)
C1	N1	C17	109.1(3)
C17	N1	Mn1	116.5(2)
C13A	N4A	Mn1A	133.5(3)
C13A	N4A	C16A	109.1(3)
C16A	N4A	Mn1A	116.9(2)
N2	C3	C2	124.3(3)
N2	C3	C4	107.5(3)
C2	C3	C4	128.2(3)
F1A	C21A	C20A	120.3(3)
F1A	C21A	C22A	117.8(3)
C20A	C21A	C22A	121.9(3)
F6A	C34A	C33A	118.8(3)
F6A	C34A	C35A	120.0(3)
C35A	C34A	C33A	121.2(3)
N4A	C13A	C12A	120.6(3)
N4A	C13A	C14A	107.4(3)
C12A	C13A	C14A	131.7(3)
F12A	C31A	C26A	119.6(3)
F12A	C31A	C30A	118.2(3)
C30A	C31A	C26A	122.1(3)
C33	C32	C7	123.1(3)
C37	C32	C7	120.7(3)
C37	C32	C33	116.1(3)
F7A	C36A	C37A	118.4(3)
F7A	C36A	C35A	119.8(3)
C35A	C36A	C37A	121.8(4)
F8A	C37A	C36A	118.4(3)
F8A	C37A	C32A	119.8(3)
C36A	C37A	C32A	121.8(3)
C5A	C4A	C3A	108.1(3)
F9A	C27A	C26A	119.7(3)
F9A	C27A	C28A	118.2(3)
C28A	C27A	C26A	122.1(3)
C6	C7	C32	116.4(3)
C8	C7	C32	117.1(3)
C8	C7	C6	126.5(3)
C31A	C26A	C27A	115.7(3)
C31A	C26A	C12A	122.5(3)
C27A	C26A	C12A	121.6(3)
F5	C33	C32	119.3(3)

Atom	Atom	Atom	Angle/°
F5	C33	C34	119.2(3)
C34	C33	C32	121.5(3)
N2	C6	C7	124.2(3)
N2	C6	C5	107.9(3)
C7	C6	C5	127.8(3)
F3A	C24A	C25A	118.1(3)
F3A	C24A	C23A	120.2(3)
C23A	C24A	C25A	121.7(3)
N3	C11	C12	124.2(3)
N3	C11	C10	107.6(3)
C12	C11	C10	128.2(3)
C24	C23	C22	116.8(3)
N3	C8	C7	124.1(3)
N3	C8	C9	108.1(3)
C7	C8	C9	127.7(3)
C37A	C32A	C7A	120.2(3)
C33A	C32A	C37A	116.0(3)
C33A	C32A	C7A	123.8(3)
C4A	C5A	C6A	108.4(3)
N1A	C17A	C16A	112.7(3)
N1A	C17A	C18A	107.7(3)
C16A	C17A	C18A	139.2(3)
F11A	C30A	C31A	118.7(3)
F11A	C30A	C29A	120.0(3)
C29A	C30A	C31A	121.2(3)
N4A	C16A	C17A	112.8(3)
N4A	C16A	C15A	108.3(3)
C17A	C16A	C15A	138.4(4)
C28	C29	C30	117.1(3)
F10A	C28A	C27A	118.9(3)
F10A	C28A	C29A	119.8(3)
C27A	C28A	C29A	121.3(3)
F9	C27	C28	118.0(3)
F9	C27	C26	120.5(3)
C28	C27	C26	121.4(3)
F8	C37	C32	119.8(3)
F8	C37	C36	118.1(3)
C36	C37	C32	122.1(3)
C10	C9	C8	107.5(3)
N2A	C3A	C4A	107.6(3)
N2A	C3A	C2A	124.2(3)
C2A	C3A	C4A	128.1(3)
C21	C20	C2	122.0(3)
C21	C20	C25	115.6(3)
C25	C20	C2	122.1(3)
F4A	C25A	C24A	118.4(3)
F4A	C25A	C20A	119.9(3)
C24A	C25A	C20A	121.7(3)
F5A	C33A	C34A	118.2(3)
F5A	C33A	C32A	119.8(3)
C32A	C33A	C34A	122.0(3)
F10	C28	C29	119.4(3)
F10	C28	C27	118.6(3)
C29	C28	C27	122.0(3)
C4	C5	C6	107.7(3)
C36A	C35A	C34A	117.2(3)
C27	C26	C12	123.7(3)
C31	C26	C27	115.9(3)
C31	C26	C12	120.4(3)
N4	C16	C17	112.9(3)
N4	C16	C15	108.0(3)
C17	C16	C15	138.7(4)
C19A	C18A	C17A	107.3(3)

Atom	Atom	Atom	Angle/°
N1A	C1A	C19A	107.2(3)
N1A	C1A	C2A	121.0(3)
C2A	C1A	C19A	131.7(3)
F1	C21	C20	119.7(3)
F1	C21	C22	118.3(3)
C22	C21	C20	122.0(3)
N1	C1	C2	120.7(3)
N1	C1	C19	107.3(3)
C2	C1	C19	131.8(3)
N3A	C11A	C12A	124.4(3)
N3A	C11A	C10A	107.6(3)
C12A	C11A	C10A	128.0(3)
C11	C12	C26	120.7(3)
C11	C12	C13	123.3(3)
C13	C12	C26	116.0(3)
F7	C36	C37	118.7(3)
F7	C36	C35	120.2(3)
C35	C36	C37	121.1(4)
N4	C13	C12	121.0(3)
N4	C13	C14	107.1(3)
C12	C13	C14	131.8(3)
C3	C2	C20	119.8(3)
C3	C2	C1	123.7(3)
C1	C2	C20	116.4(3)
C8A	C7A	C32A	115.6(3)
C6A	C7A	C32A	117.7(3)
C6A	C7A	C8A	126.7(3)
C13A	C12A	C26A	116.4(3)
C13A	C12A	C11A	123.9(3)
C11A	C12A	C26A	119.5(3)
C21A	C20A	C25A	116.2(3)
C21A	C20A	C2A	123.6(3)
C25A	C20A	C2A	119.9(3)
F6	C34	C33	118.4(3)
F6	C34	C35	120.1(3)
C35	C34	C33	121.5(4)
F2	C22	C23	119.4(3)
F2	C22	C21	118.9(3)
C21	C22	C23	121.7(4)
F12	C31	C26	120.0(3)
F12	C31	C30	117.5(3)
C30	C31	C26	122.4(3)

Atom	Atom	Atom	Angle/°
N1	C17	C16	112.8(3)
N1	C17	C18	108.0(3)
C16	C17	C18	138.6(4)
C14A	C15A	C16A	106.8(3)
F2A	C22A	C21A	119.3(3)
F2A	C22A	C23A	119.5(3)
C23A	C22A	C21A	121.1(3)
C24A	C23A	C22A	117.3(3)
F3	C24	C23	119.3(3)
F3	C24	C25	118.9(3)
C23	C24	C25	121.8(3)
N3A	C8A	C7A	123.8(3)
N3A	C8A	C9A	108.1(3)
C7A	C8A	C9A	128.0(3)
C18	C19	C1	108.4(3)
C18A	C19A	C1A	107.9(3)
O1A	C39A	C38A	111.6(3)
C9A	C10A	C11A	108.4(3)
C34	C35	C36	117.6(3)
N2A	C6A	C5A	107.5(3)
N2A	C6A	C7A	123.9(3)
C7A	C6A	C5A	128.6(3)
C3A	C2A	C20A	121.1(3)
C1A	C2A	C3A	123.6(3)
C1A	C2A	C20A	115.3(3)
O1	C39	C38	112.2(3)
C30A	C29A	C28A	117.5(3)
C9	C10	C11	108.3(3)
C5	C4	C3	108.2(3)
C19	C18	C17	107.0(3)
F11	C30	C29	119.6(3)
F11	C30	C31	119.3(3)
C31	C30	C29	121.1(3)
F4	C25	C20	119.6(3)
F4	C25	C24	118.4(3)
C24	C25	C20	122.0(3)
O2A	C40A	C41A	112.5(3)
C15	C14	C13	108.1(3)
C10A	C9A	C8A	107.5(3)
C15A	C14A	C13A	108.1(3)
O2	C40	C41	111.9(4)
C14	C15	C16	107.2(3)

Table 3: Torsion Angles in ° for **15**.

Atom	Atom	Atom	Atom	Angle/°
Mn1A	O1A	C39A	C38A	95.2(3)
Mn1A	N1A	C17A	C16A	2.0(4)
Mn1A	N1A	C17A	C18A	176.3(2)
Mn1A	N1A	C1A	C19A	-175.9(3)
Mn1A	N1A	C1A	C2A	0.5(5)
Mn1A	N3A	C11A	C12A	-4.5(5)
Mn1A	N3A	C11A	C10A	175.3(2)
Mn1A	N3A	C8A	C7A	8.1(5)
Mn1A	N3A	C8A	C9A	-175.1(2)
Mn1A	N2A	C3A	C4A	-164.9(2)
Mn1A	N2A	C3A	C2A	14.7(5)
Mn1A	N2A	C6A	C5A	165.7(2)
Mn1A	N2A	C6A	C7A	-14.2(5)
Mn1A	N4A	C13A	C12A	0.0(5)
Mn1A	N4A	C13A	C14A	174.7(3)

Atom	Atom	Atom	Atom	Angle/°
Mn1A	N4A	C16A	C17A	-2.6(4)
Mn1A	N4A	C16A	C15A	-176.3(2)
Mn1	O1	C39	C38	-97.2(4)
Mn1	N3	C11	C12	-13.7(5)
Mn1	N3	C11	C10	164.6(2)
Mn1	N3	C8	C7	13.8(5)
Mn1	N3	C8	C9	-165.5(2)
Mn1	N4	C16	C17	-1.9(4)
Mn1	N4	C16	C15	-175.8(2)
Mn1	N4	C13	C12	-2.7(5)
Mn1	N4	C13	C14	174.4(3)
Mn1	N2	C3	C2	4.2(5)
Mn1	N2	C3	C4	-175.6(2)
Mn1	N2	C6	C7	-8.6(5)
Mn1	N2	C6	C5	175.1(2)
Mn1	N1	C1	C2	1.8(5)
Mn1	N1	C1	C19	-173.3(3)
Mn1	N1	C17	C16	2.8(4)
Mn1	N1	C17	C18	175.3(2)
F9A	C27A	C26A	C31A	-179.8(3)
F9A	C27A	C26A	C12A	-3.8(5)
F9A	C27A	C28A	F10A	0.6(5)
F9A	C27A	C28A	C29A	-179.9(3)
F5	C33	C34	F6	0.3(5)
F5	C33	C34	C35	-178.8(3)
F12	C31	C30	F11	-0.8(5)
F12	C31	C30	C29	177.9(3)
F8A	C37A	C32A	C33A	-177.7(3)
F8A	C37A	C32A	C7A	2.2(5)
F9	C27	C28	F10	0.6(5)
F9	C27	C28	C29	-179.5(3)
F9	C27	C26	C12	-4.2(5)
F9	C27	C26	C31	179.1(3)
F1A	C21A	C20A	C25A	-179.8(3)
F1A	C21A	C20A	C2A	6.7(5)
F1A	C21A	C22A	F2A	-0.2(5)
F1A	C21A	C22A	C23A	-179.5(3)
F4A	C25A	C20A	C21A	178.6(3)
F4A	C25A	C20A	C2A	-7.6(5)
F6A	C34A	C33A	F5A	-0.4(5)
F6A	C34A	C33A	C32A	-179.2(3)
F6A	C34A	C35A	C36A	-179.9(3)
F12A	C31A	C26A	C27A	-177.3(3)
F12A	C31A	C26A	C12A	6.8(5)
F12A	C31A	C30A	F11A	-0.1(5)
F12A	C31A	C30A	C29A	178.4(3)
F2A	C22A	C23A	C24A	-179.0(3)
F6	C34	C35	C36	-177.5(3)
F7A	C36A	C37A	F8A	0.6(5)
F7A	C36A	C37A	C32A	-177.7(3)
F7A	C36A	C35A	C34A	177.3(3)
F1	C21	C22	F2	0.5(5)
F1	C21	C22	C23	-178.5(3)
F11A	C30A	C29A	C28A	177.7(3)
F8	C37	C36	F7	1.3(5)
F8	C37	C36	C35	-179.0(3)
F3	C24	C25	F4	0.2(5)
F3	C24	C25	C20	-179.5(3)
F3A	C24A	C25A	F4A	0.5(5)
F3A	C24A	C25A	C20A	-178.9(3)
F3A	C24A	C23A	C22A	179.8(3)
F7	C36	C35	C34	177.4(3)
F10A	C28A	C29A	C30A	179.0(3)

Atom	Atom	Atom	Atom	Angle/°
N1A	C17A	C16A	N4A	0.4(5)
N1A	C17A	C16A	C15A	171.4(4)
N1A	C17A	C18A	C19A	0.3(4)
N1A	C1A	C19A	C18A	1.2(4)
N1A	C1A	C2A	C3A	-6.5(5)
N1A	C1A	C2A	C20A	173.1(3)
N3A	C11A	C12A	C13A	-0.1(6)
N3A	C11A	C12A	C26A	-174.7(3)
N3A	C11A	C10A	C9A	0.2(4)
N3A	C8A	C9A	C10A	-1.4(4)
N3	C11	C12	C26	-177.0(3)
N3	C11	C12	C13	1.3(6)
N3	C11	C10	C9	-0.3(4)
N3	C8	C9	C10	0.1(4)
N4	C16	C17	N1	-0.6(5)
N4	C16	C17	C18	-169.8(4)
N4	C16	C15	C14	1.2(4)
N4	C13	C14	C15	-0.9(4)
N2A	C3A	C2A	C1A	-1.2(6)
N2A	C3A	C2A	C20A	179.2(3)
N2	C3	C2	C20	174.7(3)
N2	C3	C2	C1	-1.1(6)
N2	C3	C4	C5	0.4(4)
N2	C6	C5	C4	1.9(4)
N1	C1	C2	C3	-1.8(6)
N1	C1	C2	C20	-177.8(3)
N1	C1	C19	C18	2.5(4)
N1	C17	C18	C19	-2.2(4)
N4A	C13A	C12A	C26A	177.0(3)
N4A	C13A	C12A	C11A	2.3(5)
N4A	C13A	C14A	C15A	-2.3(4)
N4A	C16A	C15A	C14A	2.1(4)
C3	N2	C6	C7	174.7(3)
C3	N2	C6	C5	-1.6(4)
C21A	C20A	C2A	C3A	-68.5(5)
C21A	C20A	C2A	C1A	111.9(4)
C21A	C22A	C23A	C24A	0.3(6)
C13A	N4A	C16A	C17A	170.2(3)
C13A	N4A	C16A	C15A	-3.6(4)
C31A	C26A	C12A	C13A	68.8(5)
C31A	C26A	C12A	C11A	-116.2(4)
C31A	C30A	C29A	C28A	-0.8(6)
C32	C7	C6	N2	171.3(3)
C32	C7	C6	C5	-13.1(5)
C32	C7	C8	N3	-174.2(3)
C32	C7	C8	C9	5.1(5)
C32	C33	C34	F6	179.2(3)
C32	C33	C34	C35	0.2(6)
C32	C37	C36	F7	-178.4(3)
C32	C37	C36	C35	1.3(6)
C36A	C37A	C32A	C33A	0.5(5)
C36A	C37A	C32A	C7A	-179.6(3)
C37A	C36A	C35A	C34A	-0.7(6)
C37A	C32A	C33A	F5A	-179.8(3)
C37A	C32A	C33A	C34A	-0.9(5)
C37A	C32A	C7A	C8A	67.2(4)
C37A	C32A	C7A	C6A	-111.8(4)
C4A	C5A	C6A	N2A	-0.3(4)
C4A	C5A	C6A	C7A	179.5(3)
C4A	C3A	C2A	C1A	178.3(3)
C4A	C3A	C2A	C20A	-1.3(6)
C27A	C26A	C12A	C13A	-106.8(4)
C27A	C26A	C12A	C11A	68.1(5)

Atom	Atom	Atom	Atom	Angle/°
C27A	C28A	C29A	C30A	-0.5(6)
C7	C32	C33	F5	-1.3(5)
C7	C32	C33	C34	179.8(3)
C7	C32	C37	F8	-0.1(5)
C7	C32	C37	C36	179.6(3)
C7	C6	C5	C4	-174.3(4)
C7	C8	C9	C10	-179.2(3)
C26A	C31A	C30A	F11A	-177.5(3)
C26A	C31A	C30A	C29A	1.1(6)
C26A	C27A	C28A	F10A	-177.9(3)
C26A	C27A	C28A	C29A	1.6(6)
C33	C32	C7	C6	105.2(4)
C33	C32	C7	C8	-76.9(5)
C33	C32	C37	F8	-179.2(3)
C33	C32	C37	C36	0.5(6)
C33	C34	C35	C36	1.6(6)
C6	N2	C3	C2	-179.4(3)
C6	N2	C3	C4	0.8(4)
C6	C7	C8	N3	3.4(6)
C6	C7	C8	C9	-177.3(4)
C6	C5	C4	C3	-1.4(4)
C24A	C25A	C20A	C21A	-1.9(5)
C24A	C25A	C20A	C2A	171.8(3)
C11	N3	C8	C7	179.1(3)
C11	N3	C8	C9	-0.3(4)
C11	C12	C13	N4	6.9(6)
C11	C12	C13	C14	-169.4(4)
C23	C24	C25	F4	179.9(3)
C23	C24	C25	C20	0.2(6)
C8	N3	C11	C12	-177.9(3)
C8	N3	C11	C10	0.3(4)
C8	C7	C6	N2	-6.4(6)
C8	C7	C6	C5	169.3(4)
C8	C9	C10	C11	0.1(4)
C32A	C7A	C8A	N3A	-173.6(3)
C32A	C7A	C8A	C9A	10.3(5)
C32A	C7A	C6A	N2A	177.0(3)
C32A	C7A	C6A	C5A	-2.8(5)
C5A	C4A	C3A	N2A	0.7(4)
C5A	C4A	C3A	C2A	-178.9(3)
C17A	N1A	C1A	C19A	-1.0(4)
C17A	N1A	C1A	C2A	175.4(3)
C17A	C16A	C15A	C14A	-169.2(4)
C17A	C18A	C19A	C1A	-0.9(4)
C30A	C31A	C26A	C27A	0.0(5)
C30A	C31A	C26A	C12A	-175.9(3)
C16A	N4A	C13A	C12A	-171.0(3)
C16A	N4A	C13A	C14A	3.7(4)
C16A	C17A	C18A	C19A	172.1(5)
C16A	C15A	C14A	C13A	0.1(4)
C28A	C27A	C26A	C31A	-1.3(5)
C28A	C27A	C26A	C12A	174.6(3)
C27	C26	C12	C11	59.5(5)
C27	C26	C12	C13	-119.0(4)
C27	C26	C31	F12	-176.5(3)
C27	C26	C31	C30	1.8(5)
C37	C32	C7	C6	-73.8(4)
C37	C32	C7	C8	104.1(4)
C37	C32	C33	F5	177.8(3)
C37	C32	C33	C34	-1.2(5)
C37	C36	C35	C34	-2.3(6)
C3A	N2A	C6A	C5A	0.8(4)
C3A	N2A	C6A	C7A	-179.1(3)

Atom	Atom	Atom	Atom	Angle/°
C3A	C4A	C5A	C6A	-0.2(4)
C20	C21	C22	F2	178.9(3)
C20	C21	C22	C23	-0.2(6)
C25A	C24A	C23A	C22A	0.1(6)
C25A	C20A	C2A	C3A	118.3(4)
C25A	C20A	C2A	C1A	-61.4(5)
C33A	C34A	C35A	C36A	0.2(5)
C33A	C32A	C7A	C8A	-112.9(4)
C33A	C32A	C7A	C6A	68.1(5)
C28	C29	C30	F11	178.5(3)
C28	C29	C30	C31	-0.2(6)
C28	C27	C26	C12	174.1(3)
C28	C27	C26	C31	-2.6(5)
C35A	C34A	C33A	F5A	179.4(3)
C35A	C34A	C33A	C32A	0.6(6)
C35A	C36A	C37A	F8A	178.6(3)
C35A	C36A	C37A	C32A	0.3(6)
C26	C27	C28	F10	-177.7(3)
C26	C27	C28	C29	2.2(6)
C26	C12	C13	N4	-174.7(3)
C26	C12	C13	C14	9.0(6)
C26	C31	C30	F11	-179.1(3)
C26	C31	C30	C29	-0.4(6)
C16	N4	C13	C12	-175.4(3)
C16	N4	C13	C14	1.7(4)
C16	C17	C18	C19	167.4(5)
C18A	C17A	C16A	N4A	-171.2(4)
C18A	C17A	C16A	C15A	-0.2(9)
C1A	N1A	C17A	C16A	-173.8(3)
C1A	N1A	C17A	C18A	0.5(4)
C21	C20	C2	C3	-67.3(5)
C21	C20	C2	C1	108.8(4)
C21	C20	C25	F4	-179.9(3)
C21	C20	C25	C24	-0.2(6)
C1	N1	C17	C16	-168.7(3)
C1	N1	C17	C18	3.9(4)
C1	C19	C18	C17	-0.2(4)
C11A	N3A	C8A	C7A	-175.2(3)
C11A	N3A	C8A	C9A	1.6(4)
C11A	C10A	C9A	C8A	0.7(4)
C12	C11	C10	C9	177.9(4)
C12	C26	C31	F12	6.7(5)
C12	C26	C31	C30	-175.0(3)
C12	C13	C14	C15	175.7(4)
C13	N4	C16	C17	172.1(3)
C13	N4	C16	C15	-1.9(4)
C13	C14	C15	C16	-0.2(4)
C2	C3	C4	C5	-179.4(4)
C2	C20	C21	F1	3.9(5)
C2	C20	C21	C22	-174.5(3)
C2	C20	C25	F4	-5.2(6)
C2	C20	C25	C24	174.5(3)
C2	C1	C19	C18	-171.8(4)
C7A	C32A	C33A	F5A	0.3(5)
C7A	C32A	C33A	C34A	179.1(3)
C7A	C8A	C9A	C10A	175.2(3)
C12A	C13A	C14A	C15A	171.5(4)
C12A	C11A	C10A	C9A	-180.0(3)
C20A	C21A	C22A	F2A	177.7(3)
C20A	C21A	C22A	C23A	-1.6(6)
C22	C23	C24	F3	179.6(3)
C22	C23	C24	C25	-0.1(6)
C31	C26	C12	C11	-124.0(4)

Atom	Atom	Atom	Atom	Angle/°
C31	C26	C12	C13	57.5(5)
C17	N1	C1	C2	171.2(3)
C17	N1	C1	C19	-3.9(4)
C17	C16	C15	C14	-170.3(5)
C22A	C21A	C20A	C25A	2.4(5)
C22A	C21A	C20A	C2A	-171.1(3)
C23A	C24A	C25A	F4A	-179.8(3)
C23A	C24A	C25A	C20A	0.7(6)
C24	C23	C22	F2	-179.0(3)
C24	C23	C22	C21	0.1(6)
C8A	N3A	C11A	C12A	179.1(3)
C8A	N3A	C11A	C10A	-1.1(4)
C8A	C7A	C6A	N2A	-1.8(6)
C8A	C7A	C6A	C5A	178.3(3)
C19	C1	C2	C3	171.9(4)
C19	C1	C2	C20	-4.0(6)
C19A	C1A	C2A	C3A	168.9(4)
C19A	C1A	C2A	C20A	-11.5(6)
C10A	C11A	C12A	C13A	-179.9(3)
C10A	C11A	C12A	C26A	5.6(5)
C6A	N2A	C3A	C4A	-0.9(4)
C6A	N2A	C3A	C2A	178.7(3)
C6A	C7A	C8A	N3A	5.3(6)
C6A	C7A	C8A	C9A	-170.9(3)
C2A	C1A	C19A	C18A	-174.7(4)
C10	C11	C12	C26	5.1(6)
C10	C11	C12	C13	-176.6(4)
C4	C3	C2	C20	-5.5(6)
C4	C3	C2	C1	178.7(4)
C30	C29	C28	F10	179.1(3)
C30	C29	C28	C27	-0.7(6)
C25	C20	C21	F1	178.6(3)
C25	C20	C21	C22	0.2(6)
C25	C20	C2	C3	118.3(4)
C25	C20	C2	C1	-65.6(5)
C14A	C13A	C12A	C26A	3.8(6)
C14A	C13A	C12A	C11A	-170.9(4)
C15	C16	C17	N1	170.7(4)
C15	C16	C17	C18	1.4(9)

Table 4: Hydrogen Bond information for **15**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1	H1	O2	0.84	1.77	2.612(4)	176.5
O1A	H1A	O2A[1]	0.84	1.79	2.628(4)	177.5

––––

[1]1+x,+y,+z

Compound 16

OLEX²

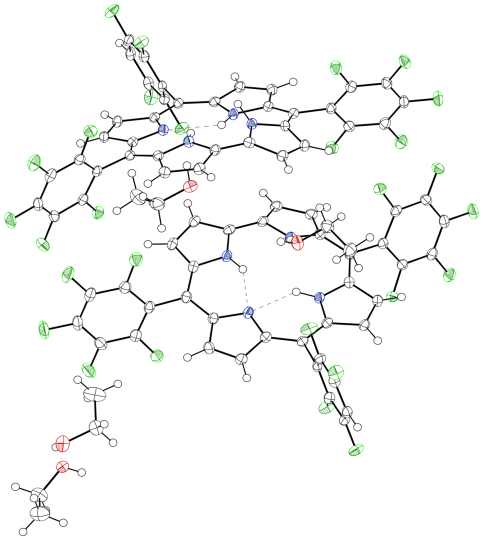
Report created with **ReportPlus**

Submitted by: **Léo Bucher**

Solved by: **Yoann Rousselin**

Sample ID: **20181016LB069**

Crystal Data and Experimental



Experimental. Single clear light red plate-shaped crystals of **Compound 16** were recrystallized from ethanol by slow evaporation. A suitable crystal 0.57 mm x 0.19 mm x 0.15 mm was selected and mounted on a MITIGEN holder oil on an Bruker D8 VENTURE diffractometer. The crystal was kept at a steady T = 100(1) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using the Intrinsic Phasing solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2018/3 of **ShelXL** (Sheldrick, 2015) using Least Squares minimization.

Crystal Data. $C_{41}H_{24}F_{14}N_4O_2$, M_r = 870.64, triclinic, P-1 (No. 2), a = 7.6090(3) Å, b = 18.3265(7) Å, c = 25.6198(10) Å, α = 94.1124(12)°, β = 90.7528(12)°, γ = 96.7722(12)°, V = 3537.7(2) Å³, T = 100(1) K, Z = 4, Z' = 2, μ(CuK$_\alpha$) = 1.354, 23668 reflections measured, 23668 unique (R_{int} = .) which were used in all calculations. The final wR_2 was 0.0945 (all data) and R_1 was 0.0361 (I > 2(I)).

Compound	**16**
CCDC	**1910515**
Formula	$C_{41}H_{24}F_{14}N_4O_2$
$D_{calc.}$/ g cm^{-3}	1.635
μ/mm^{-1}	1.354
Formula Weight	870.64
Color	clear light red
Shape	plate
Size/mm³	0.57x0.19x0.15
T/K	100(1)
Crystal System	triclinic
Space Group	P-1
a/Å	7.6090(3)
b/Å	18.3265(7)
c/Å	25.6198(10)
α/°	94.1124(12)
β/°	90.7528(12)
γ/°	96.7722(12)
V/Å³	3537.7(2)
Z	4
Z'	2
Wavelength/Å	1.54178
Radiation type	CuK$_\alpha$
Θ_{min}/°	2.881
Θ_{max}/°	66.685
Measured Refl.	23668
Independent Refl.	23668
Reflections with I > 2(I)	21454
R_{int}	.
Parameters	1126
Restraints	0
Largest Peak	0.625
Deepest Hole	-0.303
GooF	1.038
wR_2 (all data)	0.0945
wR_2	0.0910
R_1 (all data)	0.0407
R_1	0.0361

Structure Quality Indicators

Reflections:	d min (Cu) 0.84	I/σ 39.7	Rint Merged!	complete 100%
Refinement:	Shift 0.001	Max Peak 0.6	Min Peak -0.3	GooF 1.038

A clear light red plate-shaped crystal with dimensions 0.57 mm x 0.19 mm x 0.15 mm was mounted on a MITIGEN holder oil. Data were collected using a Bruker D8 VENTURE diffractometer equipped with an Oxford Cryosystems low-temperature device operating at T = 100(1) K. Data were measured using ϕ and ω scans using CuK$_\alpha$ radiation. The total number of runs and images was based on the strategy calculation from the program APEX3 (Bruker, 2015) The maximum resolution that was achieved was Θ = 66.685° (0.84 Å). The diffraction pattern was indexed. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) and the unit cell was refined using **SAINT** (Bruker, V8.38A, after 2013) on 9954 reflections, 42% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.38A, after 2013). The final completeness is 99.20 % out to 66.685° in Θ. A multi-scan absorption correction was performed using TWINABS-2012/1 (Bruker, 2012) was used for absorption correction. Final HKLF 4 output contains 78110 reflections, R_{int} = 0.0353 (64251 with I > 3sig(I), R_{int} = 0.0342). The absorption coefficient μ of this material is 1.354 mm^{-1} at this wavelength (λ = 1.542Å) and the minimum and maximum transmissions are 0.600 and 0.730. The structure was solved and the space group P-1 (# 2) determined by the **ShelXT** (Sheldrick, 2015) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model, excepted those located on nitrogen atoms which were located in Fourier difference map. Several crystals examined proved to have multiple domains. The final data crystal, while still a multiple, could be described having primarily two domains and was treated as such. Orientation matrices for the two domains were determined using the program **CELL_NOW** (Bruker, 2008) and the data were processed further using **TWINABS** (Bruker, 2008). HKLF 5 was employed, BASF specifies the fractional volume contributions of the various twin components. The crystal was refined as a non-merohedral twin with a minor twin component of 0.393(1). The value of Z' is 2. This means that there are two independent molecules in the asymmetric unit.

Table 5: Bond Lengths in Å for **Compound 16**.

Atom	Atom	Length/Å
F1	C21	1.342(2)
F2	C22	1.341(2)
F3	C23	1.330(2)
F4	C24	1.341(2)
F5	C25	1.343(2)
F6	C33	1.341(2)
F7	C34	1.345(2)
F8	C36	1.348(2)
F9	C37	1.344(2)
F10	C27	1.345(2)
F11	C28	1.341(2)
F12	C29	1.329(2)
F13	C30	1.342(2)
F14	C31	1.349(2)
N1	C1	1.383(2)
N1	C4	1.362(2)
N2	C6	1.372(2)
N2	C9	1.382(2)
N3	C11	1.372(2)
N3	C14	1.374(2)
N4	C15	1.362(2)
N4	C18	1.360(2)
C1	C2	1.445(2)
C1	C19	1.414(2)
C2	C3	1.354(3)
C3	C4	1.449(2)
C4	C5	1.420(2)
C5	C6	1.402(2)
C5	C32	1.496(2)
C6	C7	1.432(2)
C7	C8	1.363(2)
C8	C9	1.428(2)
C9	C10	1.408(2)
C10	C11	1.416(2)
C10	C26	1.479(2)
C11	C12	1.416(2)
C12	C13	1.387(2)
C13	C14	1.405(2)
C14	C15	1.411(2)
C15	C16	1.419(2)
C16	C17	1.379(3)
C17	C18	1.420(2)

Atom	Atom	Length/Å
C18	C19	1.408(2)
C19	C20	1.487(2)
C20	C21	1.392(3)
C20	C25	1.392(3)
C21	C22	1.383(3)
C22	C23	1.378(3)
C23	C24	1.378(3)
C24	C25	1.383(3)
C26	C27	1.391(3)
C26	C31	1.393(2)
C27	C28	1.381(2)
C28	C29	1.381(3)
C29	C30	1.375(3)
C30	C31	1.380(3)
C32	C33	1.390(2)
C32	C37	1.386(2)
C33	C34	1.384(2)
C34	C35	1.377(3)
C35	C36	1.371(3)
C36	C37	1.384(2)
F1A	C21A	1.345(2)
F2A	C22A	1.341(2)
F3A	C23A	1.325(2)
F4A	C24A	1.342(2)
F5A	C25A	1.345(2)
F6A	C33A	1.341(2)
F7A	C34A	1.346(2)
F8A	C36A	1.346(2)
F9A	C37A	1.347(2)
F10A	C27A	1.346(2)
F11A	C28A	1.337(2)
F12A	C29A	1.335(2)
F13A	C30A	1.343(2)
F14A	C31A	1.344(2)
N1A	C1A	1.382(2)
N1A	C4A	1.371(2)
N2A	C6A	1.365(2)
N2A	C9A	1.383(2)
N3A	C11A	1.358(2)
N3A	C14A	1.359(2)
N4A	C15A	1.377(2)
N4A	C18A	1.372(2)
C1A	C2A	1.432(2)
C1A	C19A	1.403(2)
C2A	C3A	1.363(2)

Atom	Atom	Length/Å
C3A	C4A	1.429(2)
C4A	C5A	1.404(2)
C5A	C6A	1.422(2)
C5A	C32A	1.494(2)
C6A	C7A	1.451(2)
C7A	C8A	1.353(2)
C8A	C9A	1.444(2)
C9A	C10A	1.414(2)
C10A	C11A	1.410(2)
C10A	C26A	1.485(2)
C11A	C12A	1.424(2)
C12A	C13A	1.377(3)
C13A	C14A	1.421(2)
C14A	C15A	1.411(2)
C15A	C16A	1.403(2)
C16A	C17A	1.386(3)
C17A	C18A	1.414(2)
C18A	C19A	1.412(2)
C19A	C20A	1.484(2)
C20A	C21A	1.397(2)
C20A	C25A	1.388(3)
C21A	C22A	1.378(2)
C22A	C23A	1.379(3)
C23A	C24A	1.381(3)
C24A	C25A	1.383(2)
C26A	C27A	1.389(3)
C26A	C31A	1.392(2)
C27A	C28A	1.381(3)
C28A	C29A	1.377(3)
C29A	C30A	1.377(3)
C30A	C31A	1.378(3)
C32A	C33A	1.391(2)
C32A	C37A	1.390(2)
C33A	C34A	1.384(2)
C34A	C35A	1.374(3)
C35A	C36A	1.377(3)
C36A	C37A	1.381(2)
O1	C39	1.427(2)
C38	C39	1.503(3)
O1A	C39A	1.426(2)
C38A	C39A	1.482(3)
O2	C41	1.433(2)
C40	C41	1.503(3)
O2A	C41A	1.434(2)
C40A	C41A	1.500(3)

Table 6: Bond Angles in ° for **Compound 16**.

Atom	Atom	Atom	Angle/°
C4	N1	C1	106.43(14)
C6	N2	C9	111.58(14)
C11	N3	C14	110.29(14)
C18	N4	C15	111.24(15)
N1	C1	C2	109.50(15)
N1	C1	C19	123.97(15)
C19	C1	C2	126.45(16)
C3	C2	C1	107.07(15)
C2	C3	C4	106.86(15)
N1	C4	C3	110.11(15)
N1	C4	C5	125.05(15)
C5	C4	C3	124.79(15)

Atom	Atom	Atom	Angle/°
C4	C5	C32	117.37(14)
C6	C5	C4	127.10(15)
C6	C5	C32	115.42(15)
N2	C6	C5	124.99(15)
N2	C6	C7	105.62(14)
C5	C6	C7	129.36(15)
C8	C7	C6	108.52(15)
C7	C8	C9	108.74(15)
N2	C9	C8	105.41(14)
N2	C9	C10	125.46(15)
C10	C9	C8	129.10(16)
C9	C10	C11	122.71(15)

Atom	Atom	Atom	Angle/°
C9	C10	C26	120.08(15)
C11	C10	C26	117.17(14)
N3	C11	C10	120.98(15)
N3	C11	C12	106.65(15)
C10	C11	C12	131.75(16)
C13	C12	C11	107.93(15)
C12	C13	C14	107.87(15)
N3	C14	C13	107.18(15)
N3	C14	C15	116.38(15)
C13	C14	C15	134.22(16)
N4	C15	C14	116.67(15)
N4	C15	C16	106.58(15)
C14	C15	C16	135.98(16)
C17	C16	C15	107.62(15)
C16	C17	C18	107.99(15)
N4	C18	C17	106.32(15)
N4	C18	C19	119.35(15)
C19	C18	C17	133.94(16)
C1	C19	C20	120.63(15)
C18	C19	C1	122.58(16)
C18	C19	C20	116.73(15)
C21	C20	C19	121.91(16)
C25	C20	C19	122.25(16)
C25	C20	C21	115.68(16)
F1	C21	C20	119.90(16)
F1	C21	C22	117.49(16)
C22	C21	C20	122.61(17)
F2	C22	C21	120.46(18)
F2	C22	C23	119.71(16)
C23	C22	C21	119.83(17)
F3	C23	C22	120.57(18)
F3	C23	C24	120.01(18)
C22	C23	C24	119.41(17)
F4	C24	C23	119.68(17)
F4	C24	C25	120.49(17)
C23	C24	C25	119.81(18)
F5	C25	C20	119.92(15)
F5	C25	C24	117.40(16)
C24	C25	C20	122.65(17)
C27	C26	C10	123.28(15)
C27	C26	C31	115.41(15)
C31	C26	C10	121.28(15)
F10	C27	C26	120.33(15)
F10	C27	C28	117.09(15)
C28	C27	C26	122.57(16)
F11	C28	C27	120.50(16)
F11	C28	C29	119.50(15)
C27	C28	C29	119.99(16)
F12	C29	C28	119.77(17)
F12	C29	C30	120.95(16)
C30	C29	C28	119.28(16)
F13	C30	C29	119.87(16)
F13	C30	C31	120.46(16)
C29	C30	C31	119.67(16)
F14	C31	C26	119.77(15)
F14	C31	C30	117.13(15)
C30	C31	C26	123.05(16)
C33	C32	C5	120.41(15)
C37	C32	C5	123.03(15)
C37	C32	C33	116.54(15)
F6	C33	C32	119.54(15)
F6	C33	C34	119.00(15)
C34	C33	C32	121.46(16)

Atom	Atom	Atom	Angle/°
F7	C34	C33	118.75(16)
F7	C34	C35	120.00(15)
C35	C34	C33	121.25(16)
C36	C35	C34	117.77(16)
F8	C36	C35	119.80(15)
F8	C36	C37	118.91(16)
C35	C36	C37	121.29(16)
F9	C37	C32	119.37(15)
F9	C37	C36	118.98(15)
C36	C37	C32	121.65(16)
C4A	N1A	C1A	111.84(14)
C6A	N2A	C9A	106.27(14)
C11A	N3A	C14A	111.58(14)
C18A	N4A	C15A	110.00(14)
N1A	C1A	C2A	104.99(14)
N1A	C1A	C19A	125.21(15)
C19A	C1A	C2A	129.77(16)
C3A	C2A	C1A	108.85(15)
C2A	C3A	C4A	108.54(15)
N1A	C4A	C3A	105.66(14)
N1A	C4A	C5A	124.57(15)
C5A	C4A	C3A	129.75(15)
C4A	C5A	C6A	126.81(15)
C4A	C5A	C32A	116.66(14)
C6A	C5A	C32A	116.41(14)
N2A	C6A	C5A	125.54(15)
N2A	C6A	C7A	109.94(14)
C5A	C6A	C7A	124.48(15)
C8A	C7A	C6A	107.05(15)
C7A	C8A	C9A	106.88(15)
N2A	C9A	C8A	109.85(14)
N2A	C9A	C10A	124.32(15)
C10A	C9A	C8A	125.76(15)
C9A	C10A	C26A	120.91(15)
C11A	C10A	C9A	122.82(15)
C11A	C10A	C26A	116.22(14)
N3A	C11A	C10A	118.86(15)
N3A	C11A	C12A	106.15(15)
C10A	C11A	C12A	134.46(16)
C13A	C12A	C11A	107.91(15)
C12A	C13A	C14A	107.70(15)
N3A	C14A	C13A	106.43(15)
N3A	C14A	C15A	116.54(15)
C15A	C14A	C13A	136.34(16)
N4A	C15A	C14A	115.89(15)
N4A	C15A	C16A	107.34(15)
C16A	C15A	C14A	134.87(16)
C17A	C16A	C15A	107.78(15)
C16A	C17A	C18A	108.01(15)
N4A	C18A	C17A	106.80(14)
N4A	C18A	C19A	121.10(15)
C19A	C18A	C17A	131.56(16)
C1A	C19A	C18A	123.24(15)
C1A	C19A	C20A	120.53(15)
C18A	C19A	C20A	116.22(15)
C21A	C20A	C19A	120.63(15)
C25A	C20A	C19A	123.68(15)
C25A	C20A	C21A	115.51(15)
F1A	C21A	C20A	119.76(15)
F1A	C21A	C22A	117.52(15)
C22A	C21A	C20A	122.72(16)
F2A	C22A	C21A	120.30(16)
F2A	C22A	C23A	119.69(15)

Atom	Atom	Atom	Angle/°
C21A	C22A	C23A	120.01(16)
F3A	C23A	C22A	120.24(16)
F3A	C23A	C24A	120.69(17)
C22A	C23A	C24A	119.07(16)
F4A	C24A	C23A	119.57(16)
F4A	C24A	C25A	120.46(16)
C23A	C24A	C25A	119.97(16)
F5A	C25A	C20A	120.02(15)
F5A	C25A	C24A	117.27(15)
C24A	C25A	C20A	122.70(16)
C27A	C26A	C10A	122.45(15)
C27A	C26A	C31A	115.56(15)
C31A	C26A	C10A	121.85(15)
F10A	C27A	C26A	119.90(15)
F10A	C27A	C28A	117.32(15)
C28A	C27A	C26A	122.74(16)
F11A	C28A	C27A	120.19(16)
F11A	C28A	C29A	120.10(16)
C29A	C28A	C27A	119.70(16)
F12A	C29A	C28A	119.95(17)
F12A	C29A	C30A	120.57(17)
C28A	C29A	C30A	119.48(16)
F13A	C30A	C29A	119.85(16)
F13A	C30A	C31A	120.39(17)

Atom	Atom	Atom	Angle/°
C29A	C30A	C31A	119.75(16)
F14A	C31A	C26A	119.90(15)
F14A	C31A	C30A	117.34(15)
C30A	C31A	C26A	122.73(16)
C33A	C32A	C5A	120.17(15)
C37A	C32A	C5A	123.50(15)
C37A	C32A	C33A	116.32(15)
F6A	C33A	C32A	119.71(15)
F6A	C33A	C34A	118.74(15)
C34A	C33A	C32A	121.56(16)
F7A	C34A	C33A	118.64(16)
F7A	C34A	C35A	119.95(15)
C35A	C34A	C33A	121.41(16)
C34A	C35A	C36A	117.65(16)
F8A	C36A	C35A	119.32(15)
F8A	C36A	C37A	119.37(16)
C35A	C36A	C37A	121.31(16)
F9A	C37A	C32A	119.29(15)
F9A	C37A	C36A	118.96(15)
C36A	C37A	C32A	121.74(16)
O1	C39	C38	112.84(16)
O1A	C39A	C38A	112.81(18)
O2	C41	C40	111.68(19)
O2A	C41A	C40A	112.34(16)

Table 7: Torsion Angles in ° for **Compound 16**.

Atom	Atom	Atom	Atom	Angle/°
F1	C21	C22	F2	0.2(3)
F1	C21	C22	C23	-179.90(16)
F2	C22	C23	F3	1.2(3)
F2	C22	C23	C24	-179.84(16)
F3	C23	C24	F4	0.5(3)
F3	C23	C24	C25	178.78(16)
F4	C24	C25	F5	-0.1(3)
F4	C24	C25	C20	177.81(16)
F6	C33	C34	F7	1.9(2)
F6	C33	C34	C35	-177.80(16)
F7	C34	C35	C36	178.68(15)
F8	C36	C37	F9	0.6(2)
F8	C36	C37	C32	-179.04(15)
F10	C27	C28	F11	1.4(2)
F10	C27	C28	C29	-179.36(15)
F11	C28	C29	F12	-1.4(2)
F11	C28	C29	C30	178.70(15)
F12	C29	C30	F13	-1.6(3)
F12	C29	C30	C31	179.13(15)
F13	C30	C31	F14	-1.0(2)
F13	C30	C31	C26	-178.17(15)
N1	C1	C2	C3	1.5(2)
N1	C1	C19	C18	-4.3(3)
N1	C1	C19	C20	172.66(15)
N1	C4	C5	C6	-4.4(3)
N1	C4	C5	C32	171.62(15)
N2	C6	C7	C8	1.55(19)
N2	C9	C10	C11	8.7(3)
N2	C9	C10	C26	-169.00(16)
N3	C11	C12	C13	-1.86(19)
N3	C14	C15	N4	-7.7(2)
N3	C14	C15	C16	-176.15(18)
N4	C15	C16	C17	-2.75(19)

Atom	Atom	Atom	Atom	Angle/°
N4	C18	C19	C1	-3.8(3)
N4	C18	C19	C20	179.15(15)
C1	N1	C4	C3	0.14(18)
C1	N1	C4	C5	177.73(16)
C1	C2	C3	C4	-1.37(19)
C1	C19	C20	C21	121.95(19)
C1	C19	C20	C25	-62.9(2)
C2	C1	C19	C18	172.11(17)
C2	C1	C19	C20	-11.0(3)
C2	C3	C4	N1	0.8(2)
C2	C3	C4	C5	-176.79(16)
C3	C4	C5	C6	172.83(16)
C3	C4	C5	C32	-11.1(2)
C4	N1	C1	C2	-0.99(18)
C4	N1	C1	C19	175.91(16)
C4	C5	C6	N2	-0.8(3)
C4	C5	C6	C7	176.66(17)
C4	C5	C32	C33	-77.0(2)
C4	C5	C32	C37	104.46(19)
C5	C6	C7	C8	-176.30(17)
C5	C32	C33	F6	0.7(2)
C5	C32	C33	C34	-178.35(16)
C5	C32	C37	F9	-2.5(2)
C5	C32	C37	C36	177.17(16)
C6	N2	C9	C8	3.83(19)
C6	N2	C9	C10	-174.22(16)
C6	C5	C32	C33	99.53(19)
C6	C5	C32	C37	-79.0(2)
C6	C7	C8	C9	0.7(2)
C7	C8	C9	N2	-2.74(19)
C7	C8	C9	C10	175.22(17)
C8	C9	C10	C11	-168.85(17)
C8	C9	C10	C26	13.4(3)
C9	N2	C6	C5	174.57(16)
C9	N2	C6	C7	-3.40(19)
C9	C10	C11	N3	16.6(3)
C9	C10	C11	C12	-153.08(18)
C9	C10	C26	C27	56.5(2)
C9	C10	C26	C31	-125.58(18)
C10	C11	C12	C13	168.95(18)
C10	C26	C27	F10	-2.4(2)
C10	C26	C27	C28	176.16(16)
C10	C26	C31	F14	5.2(2)
C10	C26	C31	C30	-177.73(16)
C11	N3	C14	C13	-2.76(19)
C11	N3	C14	C15	162.74(15)
C11	C10	C26	C27	-121.31(18)
C11	C10	C26	C31	56.6(2)
C11	C12	C13	C14	0.2(2)
C12	C13	C14	N3	1.52(19)
C12	C13	C14	C15	-160.25(19)
C13	C14	C15	N4	152.77(19)
C13	C14	C15	C16	-15.6(4)
C14	N3	C11	C10	-169.15(15)
C14	N3	C11	C12	2.87(19)
C14	C15	C16	C17	166.45(19)
C15	N4	C18	C17	-5.15(19)
C15	N4	C18	C19	168.64(15)
C15	C16	C17	C18	-0.3(2)
C16	C17	C18	N4	3.25(19)
C16	C17	C18	C19	-169.22(18)
C17	C18	C19	C1	167.89(18)
C17	C18	C19	C20	-9.1(3)

Atom	Atom	Atom	Atom	Angle/°
C18	N4	C15	C14	-166.65(15)
C18	N4	C15	C16	4.98(19)
C18	C19	C20	C21	-61.0(2)
C18	C19	C20	C25	114.18(19)
C19	C1	C2	C3	-175.29(17)
C19	C20	C21	F1	-5.2(3)
C19	C20	C21	C22	174.53(16)
C19	C20	C25	F5	3.4(3)
C19	C20	C25	C24	-174.43(16)
C20	C21	C22	F2	-179.57(16)
C20	C21	C22	C23	0.3(3)
C21	C20	C25	F5	178.86(15)
C21	C20	C25	C24	1.0(3)
C21	C22	C23	F3	-178.70(17)
C21	C22	C23	C24	0.3(3)
C22	C23	C24	F4	-178.50(17)
C22	C23	C24	C25	-0.2(3)
C23	C24	C25	F5	-178.38(16)
C23	C24	C25	C20	-0.5(3)
C25	C20	C21	F1	179.30(16)
C25	C20	C21	C22	-0.9(3)
C26	C10	C11	N3	-165.56(15)
C26	C10	C11	C12	24.7(3)
C26	C27	C28	F11	-177.23(15)
C26	C27	C28	C29	2.0(3)
C27	C26	C31	F14	-176.79(14)
C27	C26	C31	C30	0.3(2)
C27	C28	C29	F12	179.40(15)
C27	C28	C29	C30	-0.5(3)
C28	C29	C30	F13	178.30(15)
C28	C29	C30	C31	-0.9(3)
C29	C30	C31	F14	178.23(15)
C29	C30	C31	C26	1.1(3)
C31	C26	C27	F10	179.57(14)
C31	C26	C27	C28	-1.8(2)
C32	C5	C6	N2	-176.91(15)
C32	C5	C6	C7	0.6(3)
C32	C33	C34	F7	-179.05(15)
C32	C33	C34	C35	1.2(3)
C33	C32	C37	F9	178.90(15)
C33	C32	C37	C36	-1.5(2)
C33	C34	C35	C36	-1.6(3)
C34	C35	C36	F8	-179.40(16)
C34	C35	C36	C37	0.5(3)
C35	C36	C37	F9	-179.25(16)
C35	C36	C37	C32	1.1(3)
C37	C32	C33	F6	179.34(16)
C37	C32	C33	C34	0.3(2)
F1A	C21A	C22A	F2A	0.1(2)
F1A	C21A	C22A	C23A	-179.75(15)
F2A	C22A	C23A	F3A	0.2(3)
F2A	C22A	C23A	C24A	-178.92(15)
F3A	C23A	C24A	F4A	1.1(3)
F3A	C23A	C24A	C25A	-179.21(16)
F4A	C24A	C25A	F5A	-0.6(2)
F4A	C24A	C25A	C20A	178.54(15)
F6A	C33A	C34A	F7A	0.6(2)
F6A	C33A	C34A	C35A	-179.12(15)
F7A	C34A	C35A	C36A	178.96(15)
F8A	C36A	C37A	F9A	-0.3(2)
F8A	C36A	C37A	C32A	-179.25(15)
F10A	C27A	C28A	F11A	1.2(2)
F10A	C27A	C28A	C29A	179.46(15)

Atom	Atom	Atom	Atom	Angle/°
F11A	C28A	C29A	F12A	-1.4(3)
F11A	C28A	C29A	C30A	178.56(16)
F12A	C29A	C30A	F13A	-2.0(3)
F12A	C29A	C30A	C31A	178.61(16)
F13A	C30A	C31A	F14A	-0.5(2)
F13A	C30A	C31A	C26A	-178.56(15)
N1A	C1A	C2A	C3A	2.28(19)
N1A	C1A	C19A	C18A	-7.2(3)
N1A	C1A	C19A	C20A	171.32(15)
N1A	C4A	C5A	C6A	0.6(3)
N1A	C4A	C5A	C32A	176.33(15)
N2A	C6A	C7A	C8A	-0.49(19)
N2A	C9A	C10A	C11A	4.2(3)
N2A	C9A	C10A	C26A	-173.03(15)
N3A	C11A	C12A	C13A	-3.05(19)
N3A	C14A	C15A	N4A	8.2(2)
N3A	C14A	C15A	C16A	-153.69(19)
N4A	C15A	C16A	C17A	-1.08(19)
N4A	C18A	C19A	C1A	-17.2(3)
N4A	C18A	C19A	C20A	164.18(15)
C1A	N1A	C4A	C3A	3.63(18)
C1A	N1A	C4A	C5A	-174.59(15)
C1A	C2A	C3A	C4A	-0.2(2)
C1A	C19A	C20A	C21A	122.17(18)
C1A	C19A	C20A	C25A	-62.9(2)
C2A	C1A	C19A	C18A	170.57(17)
C2A	C1A	C19A	C20A	-10.9(3)
C2A	C3A	C4A	N1A	-2.06(19)
C2A	C3A	C4A	C5A	176.04(17)
C3A	C4A	C5A	C6A	-177.18(17)
C3A	C4A	C5A	C32A	-1.4(3)
C4A	N1A	C1A	C2A	-3.71(18)
C4A	N1A	C1A	C19A	174.55(16)
C4A	C5A	C6A	N2A	4.3(3)
C4A	C5A	C6A	C7A	-173.24(16)
C4A	C5A	C32A	C33A	-107.22(18)
C4A	C5A	C32A	C37A	73.5(2)
C5A	C6A	C7A	C8A	177.40(16)
C5A	C32A	C33A	F6A	1.1(2)
C5A	C32A	C33A	C34A	-179.02(15)
C5A	C32A	C37A	F9A	-0.9(2)
C5A	C32A	C37A	C36A	178.06(15)
C6A	N2A	C9A	C8A	1.05(18)
C6A	N2A	C9A	C10A	-175.99(16)
C6A	C5A	C32A	C33A	69.0(2)
C6A	C5A	C32A	C37A	-110.27(19)
C6A	C7A	C8A	C9A	1.09(19)
C7A	C8A	C9A	N2A	-1.37(19)
C7A	C8A	C9A	C10A	175.62(16)
C8A	C9A	C10A	C11A	-172.38(16)
C8A	C9A	C10A	C26A	10.4(3)
C9A	N2A	C6A	C5A	-178.23(16)
C9A	N2A	C6A	C7A	-0.37(18)
C9A	C10A	C11A	N3A	3.0(2)
C9A	C10A	C11A	C12A	-167.30(18)
C9A	C10A	C26A	C27A	61.9(2)
C9A	C10A	C26A	C31A	-122.57(18)
C10A	C11A	C12A	C13A	168.14(19)
C10A	C26A	C27A	F10A	-4.2(2)
C10A	C26A	C27A	C28A	173.79(16)
C10A	C26A	C31A	F14A	7.0(2)
C10A	C26A	C31A	C30A	-174.96(16)
C11A	N3A	C14A	C13A	-4.78(19)

Atom	Atom	Atom	Atom	Angle/°
C11A	N3A	C14A	C15A	167.27(15)
C11A	C10A	C26A	C27A	-115.45(18)
C11A	C10A	C26A	C31A	60.0(2)
C11A	C12A	C13A	C14A	0.2(2)
C12A	C13A	C14A	N3A	2.7(2)
C12A	C13A	C14A	C15A	-167.0(2)
C13A	C14A	C15A	N4A	177.13(19)
C13A	C14A	C15A	C16A	15.2(4)
C14A	N3A	C11A	C10A	-167.92(15)
C14A	N3A	C11A	C12A	4.90(19)
C14A	C15A	C16A	C17A	161.90(19)
C15A	N4A	C18A	C17A	-2.57(19)
C15A	N4A	C18A	C19A	169.88(15)
C15A	C16A	C17A	C18A	-0.5(2)
C16A	C17A	C18A	N4A	1.86(19)
C16A	C17A	C18A	C19A	-169.49(18)
C17A	C18A	C19A	C1A	153.12(18)
C17A	C18A	C19A	C20A	-25.5(3)
C18A	N4A	C15A	C14A	-164.37(15)
C18A	N4A	C15A	C16A	2.30(19)
C18A	C19A	C20A	C21A	-59.2(2)
C18A	C19A	C20A	C25A	115.76(19)
C19A	C1A	C2A	C3A	-175.87(17)
C19A	C20A	C21A	F1A	-6.1(2)
C19A	C20A	C21A	C22A	174.78(16)
C19A	C20A	C25A	F5A	5.3(3)
C19A	C20A	C25A	C24A	-173.78(16)
C20A	C21A	C22A	F2A	179.24(15)
C20A	C21A	C22A	C23A	-0.6(3)
C21A	C20A	C25A	F5A	-179.54(14)
C21A	C20A	C25A	C24A	1.4(3)
C21A	C22A	C23A	F3A	-179.99(16)
C21A	C22A	C23A	C24A	0.9(3)
C22A	C23A	C24A	F4A	-179.73(15)
C22A	C23A	C24A	C25A	-0.1(3)
C23A	C24A	C25A	F5A	179.79(15)
C23A	C24A	C25A	C20A	-1.1(3)
C25A	C20A	C21A	F1A	178.61(15)
C25A	C20A	C21A	C22A	-0.6(3)
C26A	C10A	C11A	N3A	-179.63(15)
C26A	C10A	C11A	C12A	10.0(3)
C26A	C27A	C28A	F11A	-176.82(15)
C26A	C27A	C28A	C29A	1.5(3)
C27A	C26A	C31A	F14A	-177.18(14)
C27A	C26A	C31A	C30A	0.8(2)
C27A	C28A	C29A	F12A	-179.70(16)
C27A	C28A	C29A	C30A	0.3(3)
C28A	C29A	C30A	F13A	178.02(16)
C28A	C29A	C30A	C31A	-1.4(3)
C29A	C30A	C31A	F14A	178.85(15)
C29A	C30A	C31A	C26A	0.8(3)
C31A	C26A	C27A	F10A	-179.90(14)
C31A	C26A	C27A	C28A	-2.0(2)
C32A	C5A	C6A	N2A	-171.43(15)
C32A	C5A	C6A	C7A	11.0(2)
C32A	C33A	C34A	F7A	-179.25(15)
C32A	C33A	C34A	C35A	1.0(3)
C33A	C32A	C37A	F9A	179.86(14)
C33A	C32A	C37A	C36A	-1.2(2)
C33A	C34A	C35A	C36A	-1.3(3)
C34A	C35A	C36A	F8A	-179.47(15)
C34A	C35A	C36A	C37A	0.4(3)
C35A	C36A	C37A	F9A	179.86(15)

Atom	Atom	Atom	Atom	Angle/°
C35A	C36A	C37A	C32A	0.9(3)
C37A	C32A	C33A	F6A	-179.61(14)
C37A	C32A	C33A	C34A	0.3(2)

Table 8: Hydrogen Bond information for **Compound 16**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N2	H2	N1	0.89(2)	2.33(2)	2.937(2)	125.7(17)
N3	H3	O1	0.86(2)	1.89(2)	2.7541(19)	173(2)
N4	H4	N1	0.85(2)	1.91(2)	2.625(2)	140(2)
N1A	H1A	N2A	0.87(2)	2.32(2)	2.933(2)	127.9(18)
N3A	H3AA	N2A	0.84(2)	1.95(2)	2.631(2)	138(2)
N4A	H4A	O1A[1]	0.93(2)	1.82(2)	2.7522(19)	174.2(19)
O1	H1	O2[2]	0.84	1.87	2.7003(18)	169.8
O1A	H1AA	O2A[2]	0.84	1.88	2.7029(19)	167.7

––––

[1]2-x,1-y,1-z; [2]1-x,1-y,1-z

Compound 17

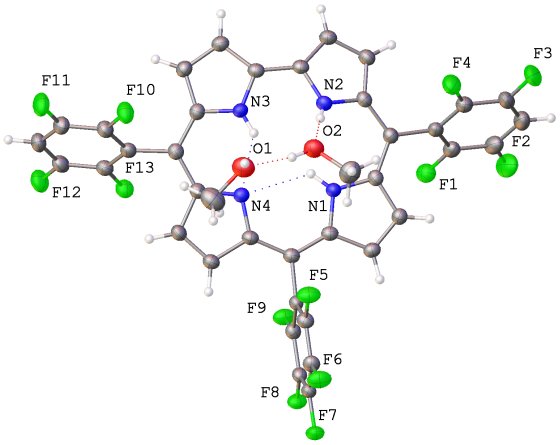
Report created with **ReportPlus**

Submitted by: **Léo Bucher**

Solved by: **Yoann Rousselin**

Sample ID: **20181010LB056**

Crystal Data and Experimental



Experimental. Single clear light violet plate-shaped crystals of **Compound 17** were recrystallized from methanol by slow evaporation. A suitable crystal 0.62 mm x 0.30 mm x 0.15 mm was selected and mounted on a MITIGEN holder oil on a Bruker D8 VENTURE diffractometer. The crystal was kept at a steady T = 100(1) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using the Intrinsic Phasing solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2018/3 of **ShelXL** (Sheldrick, 2015) using Least Squares minimization.

Crystal Data. $C_{39}H_{21}F_{13}N_4O_2$, M_r = 824.60, monoclinic, $P2_1/c$ (No. 14), a = 15.9471(7) Å, b = 7.3379(3) Å, c = 29.9200(12) Å, β = 104.5867(14)°, α = γ = 90°, V = 3388.3(2) Å^3, T = 100(1) K, Z = 4, Z' = 1, μ(CuK$_\alpha$) = 1.333, 11273 reflections measured, 11273 unique (R_{int} = .) which were used in all calculations. The final wR_2 was 0.1431 (all data) and R_1 was 0.0525 (I > 2(I)).

Compound	**17**
CCDC	**1910516**
Formula	$C_{39}H_{21}F_{13}N_4O_2$
$D_{calc.}$/ g cm^{-3}	1.616
μ/mm^{-1}	1.333
Formula Weight	824.60
Color	clear light violet
Shape	plate
Size/mm^3	0.62x0.30x0.15
T/K	100(1)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	15.9471(7)
b/Å	7.3379(3)
c/Å	29.9200(12)
α/°	90
β/°	104.5867(14)
γ/°	90
V/Å^3	3388.3(2)
Z	4
Z'	1
Wavelength/Å	1.54178
Radiation type	CuK$_\alpha$
Θ_{min}/°	2.863
Θ_{max}/°	66.762
Measured Refl.	11273
Independent Refl.	11273
Reflections with I > 2(I)	10369
R_{int}	.
Parameters	537
Restraints	0
Largest Peak	0.360
Deepest Hole	-0.315
GooF	1.117
wR_2 (all data)	0.1431
wR_2	0.1404
R_1 (all data)	0.0560
R_1	0.0525

Structure Quality Indicators

Reflections:	d min (Cu) 0.84	I/σ 34.9	Rint Merged!	complete 100%
Refinement:	Shift 0.000	Max Peak 0.4	Min Peak -0.3	GooF 1.117

A clear light violet plate-shaped crystal with dimensions 0.62 mm x 0.30 mm x 0.15 mm was mounted on a MITIGEN holder oil. Data were collected using a Bruker D8 VENTURE diffractometer equipped with an Oxford Cryosystems low-temperature device operating at T = 100(1) K. Data were measured using ϕ and ω scans' using CuK_α radiation. The total number of runs and images was based on the strategy calculation from the program APEX3 (Bruker, 2015) The maximum resolution that was achieved was Θ = 66.762° (0.84 Å). The diffraction pattern was indexed. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) and the unit cell was refined using **SAINT** (Bruker, V8.38A, after 2013) on 9877 reflections, 88% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.38A, after 2013). The final completeness is 99.80 % out to 66.762° in Θ. A multi-scan absorption correction was performed using TWINABS-2012/1 (Bruker,2012) was used for absorption correction. Final HKLF 4 output contains 94043 reflections, R_{int} = 0.0595 (69025 with I > 3sig(I), R_{int} = 0.0576). The absorption coefficient μ of this material is 1.333 mm^{-1} at this wavelength (λ = 1.542Å) and the minimum and maximum transmissions are 0.470 and 0.700. The structure was solved and the space group $P2_1/c$ (# 14) determined by the **ShelXT** (Sheldrick, 2015) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model, excepted those located on nitrogen atoms which were located in Fourier difference map. There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 4 and Z' is 1. Several crystals examined proved to have multiple domains. The final data crystal, while still a multiple, could be described having primarily two domains and was treated as such. Orientation matrices for the two domains were determined using the program **CELL_NOW** (Bruker, 2008) and the data were processed further using **TWINABS** (Bruker, 2008). HKLF 5 was employed, BASF specifies the fractional volume contributions of the various twin components. The crystal was refined as a non-merohedral twin with a minor twin component of 0.116(1).

Table 9: Bond Lengths in Å for **Compound 17**.

Atom	Atom	Length/Å
F1	C25	1.344(3)
F2	C24	1.349(4)
F3	C22	1.352(4)
F4	C21	1.343(4)
F5	C27	1.338(3)
F6	C28	1.339(3)
F7	C29	1.340(3)
F8	C30	1.341(3)
F9	C31	1.338(3)
F10	C33	1.341(3)
F11	C34	1.346(3)
F12	C36	1.347(3)
F13	C37	1.344(3)
N1	C1	1.381(3)
N1	C17	1.371(3)
N2	C3	1.376(3)
N2	C6	1.372(3)
N3	C7	1.367(3)
N3	C10	1.359(3)
N4	C12	1.381(3)
N4	C15	1.365(3)

Atom	Atom	Length/Å
C1	C2	1.411(4)
C1	C19	1.422(4)
C2	C3	1.410(4)
C2	C20	1.486(4)
C3	C4	1.413(4)
C4	C5	1.377(4)
C5	C6	1.415(4)
C6	C7	1.411(4)
C7	C8	1.414(4)
C8	C9	1.380(4)
C9	C10	1.423(4)
C10	C11	1.410(4)
C11	C12	1.408(4)
C11	C32	1.485(4)
C12	C13	1.446(4)
C13	C14	1.354(4)
C14	C15	1.448(4)
C15	C16	1.413(4)
C16	C17	1.403(4)
C16	C26	1.492(3)
C17	C18	1.423(4)

Atom	Atom	Length/Å
C18	C19	1.368(4)
C20	C21	1.391(4)
C20	C25	1.393(4)
C21	C22	1.384(4)
C22	C23	1.376(5)
C23	C24	1.369(5)
C24	C25	1.385(4)
C26	C27	1.388(4)
C26	C31	1.387(4)
C27	C28	1.381(4)
C28	C29	1.372(4)
C29	C30	1.379(4)
C30	C31	1.382(4)
C32	C33	1.389(4)
C32	C37	1.393(4)
C33	C34	1.380(4)
C34	C35	1.376(4)
C35	C36	1.369(4)
C36	C37	1.385(4)
O1	C38	1.409(4)
O2	C39	1.424(4)

Table 10: Bond Angles in ° for **Compound 17**.

Atom	Atom	Atom	Angle/°
C17	N1	C1	111.1(2)
C6	N2	C3	110.4(2)
C10	N3	C7	111.6(2)
C15	N4	C12	106.8(2)
N1	C1	C2	125.9(2)
N1	C1	C19	105.7(2)
C2	C1	C19	128.4(2)
C1	C2	C20	117.5(2)
C3	C2	C1	123.2(2)
C3	C2	C20	119.1(2)
N2	C3	C2	120.5(2)
N2	C3	C4	106.3(2)
C2	C3	C4	132.1(2)
C5	C4	C3	108.6(2)
C4	C5	C6	107.7(2)
N2	C6	C5	106.9(2)
N2	C6	C7	116.4(2)
C7	C6	C5	134.5(2)
N3	C7	C6	116.8(2)
N3	C7	C8	106.4(2)
C6	C7	C8	136.1(2)
C9	C8	C7	107.7(2)
C8	C9	C10	108.2(2)
N3	C10	C9	105.9(2)
N3	C10	C11	119.8(2)
C11	C10	C9	133.9(2)
C10	C11	C32	116.8(2)
C12	C11	C10	122.8(2)
C12	C11	C32	120.4(2)
N4	C12	C11	124.3(2)
N4	C12	C13	109.1(2)
C11	C12	C13	126.6(2)
C14	C13	C12	107.5(2)
C13	C14	C15	106.7(2)
N4	C15	C14	109.9(2)
N4	C15	C16	124.6(2)
C16	C15	C14	125.5(2)
C15	C16	C26	118.2(2)
C17	C16	C15	126.8(2)
C17	C16	C26	115.0(2)
N1	C17	C16	125.2(2)
N1	C17	C18	106.3(2)
C16	C17	C18	128.6(2)
C19	C18	C17	108.2(2)
C18	C19	C1	108.7(2)
C21	C20	C2	122.2(3)
C21	C20	C25	116.3(3)
C25	C20	C2	121.5(2)
F4	C21	C20	120.1(2)
F4	C21	C22	118.4(3)
C22	C21	C20	121.5(3)
F3	C22	C21	118.5(3)
F3	C22	C23	120.2(3)
C23	C22	C21	121.3(3)
C24	C23	C22	118.0(3)
F2	C24	C23	120.5(3)
F2	C24	C25	118.3(3)
C23	C24	C25	121.2(3)
F1	C25	C20	120.7(2)
F1	C25	C24	117.7(3)
C24	C25	C20	121.7(3)
C27	C26	C16	121.0(2)
C31	C26	C16	122.7(2)
C31	C26	C27	116.3(2)
F5	C27	C26	119.6(2)
F5	C27	C28	118.0(2)
C28	C27	C26	122.4(2)
F6	C28	C27	120.4(2)
F6	C28	C29	119.8(2)
C29	C28	C27	119.8(2)
F7	C29	C28	120.5(2)
F7	C29	C30	119.9(2)
C28	C29	C30	119.7(2)
F8	C30	C29	119.6(2)
F8	C30	C31	120.8(2)
C29	C30	C31	119.6(2)
F9	C31	C26	119.9(2)
F9	C31	C30	117.8(2)
C30	C31	C26	122.3(2)
C33	C32	C11	121.4(2)
C33	C32	C37	116.1(2)
C37	C32	C11	122.5(2)
F10	C33	C32	120.0(2)
F10	C33	C34	117.9(2)
C34	C33	C32	122.1(3)
F11	C34	C33	118.7(3)
F11	C34	C35	120.3(3)
C35	C34	C33	121.0(3)
C36	C35	C34	117.9(3)
F12	C36	C35	119.9(3)
F12	C36	C37	118.6(3)
C35	C36	C37	121.5(3)

Atom	Atom	Atom	Angle/°
F13	C37	C32	120.1(2)
F13	C37	C36	118.4(2)
C36	C37	C32	121.4(3)

Table 11: Torsion Angles in ° for **Compound 17**.

Atom	Atom	Atom	Atom	Angle/°
F2	C24	C25	F1	-1.0(4)
F2	C24	C25	C20	179.5(3)
F3	C22	C23	C24	-179.7(3)
F4	C21	C22	F3	-1.1(4)
F4	C21	C22	C23	178.2(3)
F5	C27	C28	F6	1.5(4)
F5	C27	C28	C29	-179.4(2)
F6	C28	C29	F7	-1.7(4)
F6	C28	C29	C30	178.3(2)
F7	C29	C30	F8	-0.1(4)
F7	C29	C30	C31	-179.9(2)
F8	C30	C31	F9	0.5(4)
F8	C30	C31	C26	-178.9(2)
F10	C33	C34	F11	1.5(4)
F10	C33	C34	C35	-178.6(3)
F11	C34	C35	C36	-179.4(3)
F12	C36	C37	F13	-0.1(4)
F12	C36	C37	C32	178.7(2)
N1	C1	C2	C3	7.5(4)
N1	C1	C2	C20	-167.3(2)
N1	C1	C19	C18	-0.7(3)
N1	C17	C18	C19	0.9(3)
N2	C3	C4	C5	-2.7(3)
N2	C6	C7	N3	-4.9(3)
N2	C6	C7	C8	-173.6(3)
N3	C7	C8	C9	-1.7(3)
N3	C10	C11	C12	-6.4(4)
N3	C10	C11	C32	175.0(2)
N4	C12	C13	C14	0.7(3)
N4	C15	C16	C17	-0.2(4)
N4	C15	C16	C26	177.8(2)
C1	N1	C17	C16	177.3(2)
C1	N1	C17	C18	-1.4(3)
C1	C2	C3	N2	12.8(4)
C1	C2	C3	C4	-153.8(3)
C1	C2	C20	C21	-126.9(3)
C1	C2	C20	C25	52.3(4)
C2	C1	C19	C18	178.7(3)
C2	C3	C4	C5	165.3(3)
C2	C20	C21	F4	-0.3(4)
C2	C20	C21	C22	178.1(3)
C2	C20	C25	F1	2.9(4)
C2	C20	C25	C24	-177.6(3)
C3	N2	C6	C5	-3.3(3)
C3	N2	C6	C7	162.4(2)
C3	C2	C20	C21	58.1(4)
C3	C2	C20	C25	-122.8(3)
C3	C4	C5	C6	0.7(3)
C4	C5	C6	N2	1.5(3)
C4	C5	C6	C7	-160.4(3)
C5	C6	C7	N3	155.7(3)
C5	C6	C7	C8	-13.0(5)
C6	N2	C3	C2	-165.9(2)
C6	N2	C3	C4	3.7(3)
C6	C7	C8	C9	167.8(3)
C7	N3	C10	C9	-4.0(3)

Atom	Atom	Atom	Atom	Angle/°
C7	N3	C10	C11	169.9(2)
C7	C8	C9	C10	-0.7(3)
C8	C9	C10	N3	2.9(3)
C8	C9	C10	C11	-169.8(3)
C9	C10	C11	C12	165.5(3)
C9	C10	C11	C32	-13.1(4)
C10	N3	C7	C6	-168.2(2)
C10	N3	C7	C8	3.6(3)
C10	C11	C12	N4	-5.6(4)
C10	C11	C12	C13	172.4(3)
C10	C11	C32	C33	-58.6(3)
C10	C11	C32	C37	118.0(3)
C11	C12	C13	C14	-177.6(3)
C11	C32	C33	F10	-5.6(4)
C11	C32	C33	C34	175.7(3)
C11	C32	C37	F13	3.2(4)
C11	C32	C37	C36	-175.6(2)
C12	N4	C15	C14	-0.5(3)
C12	N4	C15	C16	177.9(2)
C12	C11	C32	C33	122.8(3)
C12	C11	C32	C37	-60.6(4)
C12	C13	C14	C15	-0.9(3)
C13	C14	C15	N4	0.9(3)
C13	C14	C15	C16	-177.5(3)
C14	C15	C16	C17	177.9(2)
C14	C15	C16	C26	-4.1(4)
C15	N4	C12	C11	178.2(2)
C15	N4	C12	C13	-0.1(3)
C15	C16	C17	N1	0.3(4)
C15	C16	C17	C18	178.7(3)
C15	C16	C26	C27	-92.5(3)
C15	C16	C26	C31	89.7(3)
C16	C17	C18	C19	-177.7(2)
C16	C26	C27	F5	2.4(4)
C16	C26	C27	C28	-177.6(2)
C16	C26	C31	F9	-2.6(4)
C16	C26	C31	C30	176.8(2)
C17	N1	C1	C2	-178.2(2)
C17	N1	C1	C19	1.3(3)
C17	C16	C26	C27	85.8(3)
C17	C16	C26	C31	-92.0(3)
C17	C18	C19	C1	-0.1(3)
C19	C1	C2	C3	-171.8(3)
C19	C1	C2	C20	13.3(4)
C20	C2	C3	N2	-172.4(2)
C20	C2	C3	C4	21.0(4)
C20	C21	C22	F3	-179.6(3)
C20	C21	C22	C23	-0.2(5)
C21	C20	C25	F1	-177.9(2)
C21	C20	C25	C24	1.5(4)
C21	C22	C23	C24	1.0(5)
C22	C23	C24	F2	179.2(3)
C22	C23	C24	C25	-0.5(5)
C23	C24	C25	F1	178.6(3)
C23	C24	C25	C20	-0.8(5)
C25	C20	C21	F4	-179.5(2)
C25	C20	C21	C22	-1.0(4)
C26	C16	C17	N1	-177.8(2)
C26	C16	C17	C18	0.6(4)
C26	C27	C28	F6	-178.5(2)
C26	C27	C28	C29	0.6(4)
C27	C26	C31	F9	179.6(2)
C27	C26	C31	C30	-1.0(4)

Atom	Atom	Atom	Atom	Angle/°
C27	C28	C29	F7	179.2(2)
C27	C28	C29	C30	-0.8(4)
C28	C29	C30	F8	179.9(2)
C28	C29	C30	C31	0.1(4)
C29	C30	C31	F9	-179.8(2)
C29	C30	C31	C26	0.8(4)
C31	C26	C27	F5	-179.7(2)
C31	C26	C27	C28	0.3(4)
C32	C11	C12	N4	173.0(2)
C32	C11	C12	C13	-9.0(4)
C32	C33	C34	F11	-179.7(2)
C32	C33	C34	C35	0.2(4)
C33	C32	C37	F13	180.0(2)
C33	C32	C37	C36	1.2(4)
C33	C34	C35	C36	0.7(4)
C34	C35	C36	F12	-179.7(3)
C34	C35	C36	C37	-0.6(4)
C35	C36	C37	F13	-179.1(2)
C35	C36	C37	C32	-0.3(4)
C37	C32	C33	F10	177.7(2)
C37	C32	C33	C34	-1.1(4)

Table 12: Hydrogen Bond information for **Compound 17**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N1	H1	N4	0.87(3)	2.31(3)	2.910(3)	126(3)
N2	H2	O2	0.82(3)	1.97(3)	2.788(3)	173(3)
N3	H3	N4	0.82(3)	1.99(3)	2.655(3)	137(3)
O1	H1A	N4[1]	0.84	2.60	3.386(3)	157.0
O2	H2A	O1	0.84	1.90	2.733(3)	169.3

––––

[1]+x,1+y,+z

Compound 19

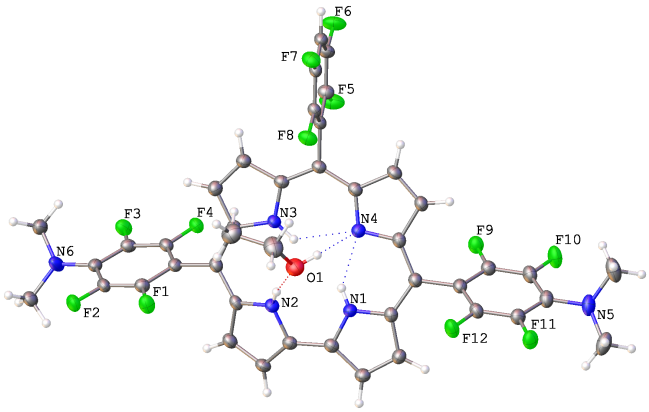
Report created with **ReportPlus**

Submitted by: **Léo Bucher**

Solved by: **Yoann Rousselin**

Sample ID: **20181018LB058**

Crystal Data and Experimental



Experimental. Single clear light red plate-shaped crystals of **Compound 19** were recrystallized from ethanol by slow evaporation. A suitable crystal 0.57 mm x 0.37 mm x 0.18 mm was selected and mounted on a MITIGEN holder oil on a Bruker D8 VENTURE diffractometer. The crystal was kept at a steady T = 100(1) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using the Intrinsic Phasing solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2018/3 of **ShelXL** (Sheldrick, 2015) using Least Squares minimization.

Crystal Data. $C_{43}H_{30}F_{12}N_6O$, M_r = 874.73, monoclinic, $P2_1/n$ (No. 14), a = 20.6155(9) Å, b = 7.3748(3) Å, c = 24.8188(11) Å, β = 91.5372(16)°, α = γ = 90°, V = 3772.0(3) Å^3, T = 100(1) K, Z = 4, Z' = 1, μ(CuK$_\alpha$) = 1.188, 11209 reflections measured, 11209 unique (R_{int} = .) which were used in all calculations. The final wR_2 was 0.1210 (all data) and R_1 was 0.0439 (I > 2(I)).

Compound	**19**
CCDC	**1910517**
Formula	$C_{43}H_{30}F_{12}N_6O$
$D_{calc.}$/ g cm^{-3}	1.540
μ/mm^{-1}	1.188
Formula Weight	874.73
Colour	clear light red
Shape	plate
Size/mm^3	0.57x0.37x0.18
T/K	100(1)
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	20.6155(9)
b/Å	7.3748(3)
c/Å	24.8188(11)
α/°	90
β/°	91.5372(16)
γ/°	90
V/Å^3	3772.0(3)
Z	4
Z'	1
Wavelength/Å	1.54178
Radiation type	CuK$_\alpha$
Θ_{min}/°	2.750
Θ_{max}/°	66.633
Measured Refl.	11209
Independent Refl.	11209
Reflections with I > 2(I)	10026
R_{int}	.
Parameters	575
Restraints	0
Largest Peak	0.306
Deepest Hole	-0.229
GooF	1.031
wR_2 (all data)	0.1210
wR_2	0.1161
R_1 (all data)	0.0491
R_1	0.0439

Structure Quality Indicators

Reflections:	d min (Cu) 0.84	I/σ 35.3	Rint Merged!	complete 99%
Refinement:	Shift 0.001	Max Peak 0.3	Min Peak -0.2	GooF 1.031

A clear light red plate-shaped crystal with dimensions 0.57 mm x 0.37mm x 0.18 mm was mounted on a MITIGEN holder oil. Data were collected using a Bruker D8 VENTURE diffractometer equipped with an Oxford Cryosystems low-temperature device operating at T = 100(1) K. Data were measured using ϕ and ω scans' using CuK_α radiation. The total number of runs and images was based on the strategy calculation from the program APEX3 (Bruker, 2015) The maximum resolution that was achieved was Θ = 66.633° (0.84 Å). The diffraction pattern was indexed. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) and the unit cell was refined using **SAINT** (Bruker, V8.38A, after 2013) on 9816 reflections, 88% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.38A, after 2013). The final completeness is 98.00 % out to 66.633° in Θ. A multi-scan absorption correction was performed using **TWINABS-2012/1** (Bruker, 2012) was used for absorption correction. Final HKLF 4 output contains 43010 reflections, R_{int} = 0.0431 (33444 with I > 3sig(I), R_{int} = 0.0419). The absorption coefficient μ of this material is 1.188 mm^{-1} at this wavelength (λ = 1.542Å) and the minimum and maximum transmissions are 0.510 and 0.680. The structure was solved and the space group $P2_1/n$ (# 14) determined by the **ShelXT** (Sheldrick, 2015) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model, excepted those located on nitrogen atoms which were located in Fourier difference map. Several crystals examined proved to have multiple domains. The final data crystal, while still a multiple, could be described having primarily two domains and was treated as such. Orientation matrices for the two domains were determined using the program **CELL_NOW** (Bruker, 2008) and the data were processed further using **TWINABS** (Bruker, 2008). HKLF 5 was employed, BASF specifies the fractional volume contributions of the various twin components. The crystal was refined as a non-merohedral twin with a minor twin component of 0.291(1).

Table 13: Bond Lengths in Å for **Compound 19**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	C29	1.350(3)	C2	C3	1.379(3)
F2	C30	1.350(3)	C3	C4	1.413(3)
F3	C32	1.352(3)	C4	C5	1.415(3)
F4	C33	1.350(2)	C5	C6	1.408(3)
F5	C37	1.343(3)	C6	C7	1.382(3)
F6	C38	1.343(3)	C7	C8	1.414(3)
F7	C40	1.350(2)	C8	C9	1.411(3)
F8	C41	1.340(3)	C9	C10	1.405(3)
F9	C25	1.344(3)	C9	C28	1.480(3)
F10	C24	1.352(3)	C10	C11	1.427(3)
F11	C22	1.351(3)	C11	C12	1.366(3)
F12	C21	1.348(3)	C12	C13	1.430(3)
N1	C1	1.358(3)	C13	C14	1.401(3)
N1	C4	1.356(3)	C14	C15	1.411(3)
C42	C43	1.500(4)	C14	C36	1.499(3)
N2	C5	1.378(3)	C15	C16	1.442(3)
N2	C8	1.376(3)	C16	C17	1.352(3)
N3	C10	1.379(3)	C17	C18	1.437(3)
N3	C13	1.372(3)	C18	C19	1.416(3)
N4	C15	1.371(3)	C19	C20	1.490(3)
N4	C18	1.390(3)	C20	C21	1.388(3)
N5	C23	1.398(3)	C20	C25	1.393(3)
N5	C26	1.461(3)	C21	C22	1.385(3)
N5	C27	1.462(4)	C22	C23	1.394(3)
N6	C31	1.382(3)	C23	C24	1.400(3)
N6	C34	1.435(3)	C24	C25	1.382(3)
N6	C35	1.444(3)	C28	C29	1.392(3)
C1	C2	1.420(3)	C28	C33	1.392(3)
C1	C19	1.406(3)	C29	C30	1.374(3)

Atom	Atom	Length/Å
C30	C31	1.395(3)
C31	C32	1.396(3)
C32	C33	1.377(3)
C36	C37	1.383(3)
C36	C41	1.387(3)

Atom	Atom	Length/Å
C37	C38	1.385(3)
C38	C39	1.372(3)
C39	C40	1.371(3)
C40	C41	1.387(3)
O1	C43	1.427(3)

Table 14: Bond Angles in ° for **Compound 19**.

Atom	Atom	Atom	Angle/°
C4	N1	C1	112.61(19)
C8	N2	C5	110.27(18)
C13	N3	C10	111.63(18)
C15	N4	C18	106.32(17)
C23	N5	C26	118.4(2)
C23	N5	C27	116.5(2)
C26	N5	C27	113.7(2)
C31	N6	C34	121.82(19)
C31	N6	C35	121.44(19)
C34	N6	C35	116.74(18)
N1	C1	C2	105.47(19)
N1	C1	C19	119.58(19)
C19	C1	C2	134.7(2)
C3	C2	C1	107.9(2)
C2	C3	C4	108.21(19)
N1	C4	C3	105.70(19)
N1	C4	C5	116.49(19)
C3	C4	C5	137.4(2)
N2	C5	C4	115.51(19)
N2	C5	C6	107.03(19)
C6	C5	C4	135.4(2)
C7	C6	C5	107.73(19)
C6	C7	C8	108.53(19)
N2	C8	C7	106.32(18)
N2	C8	C9	121.01(19)
C9	C8	C7	131.8(2)
C8	C9	C28	117.87(19)
C10	C9	C8	123.43(19)
C10	C9	C28	118.61(19)
N3	C10	C9	125.86(19)
N3	C10	C11	105.53(18)
C9	C10	C11	128.6(2)
C12	C11	C10	108.6(2)
C11	C12	C13	108.54(19)
N3	C13	C12	105.63(18)
N3	C13	C14	124.70(19)
C14	C13	C12	129.66(19)
C13	C14	C15	126.69(19)
C13	C14	C36	115.82(18)
C15	C14	C36	117.46(18)
N4	C15	C14	124.91(19)
N4	C15	C16	109.63(18)
C14	C15	C16	125.45(19)
C17	C16	C15	107.42(19)
C16	C17	C18	107.23(19)
N4	C18	C17	109.40(18)
N4	C18	C19	124.39(19)
C19	C18	C17	126.2(2)
C1	C19	C18	122.8(2)
C1	C19	C20	117.99(19)
C18	C19	C20	119.23(19)
C21	C20	C19	122.4(2)

Atom	Atom	Atom	Angle/°
C21	C20	C25	114.9(2)
C25	C20	C19	122.7(2)
F12	C21	C20	119.88(19)
F12	C21	C22	117.0(2)
C22	C21	C20	123.1(2)
F11	C22	C21	117.5(2)
F11	C22	C23	120.2(2)
C21	C22	C23	122.3(2)
N5	C23	C24	119.5(2)
C22	C23	N5	125.9(2)
C22	C23	C24	114.5(2)
F10	C24	C23	119.0(2)
F10	C24	C25	118.1(2)
C25	C24	C23	122.9(2)
F9	C25	C20	120.07(19)
F9	C25	C24	117.6(2)
C24	C25	C20	122.3(2)
C29	C28	C9	122.6(2)
C33	C28	C9	122.8(2)
C33	C28	C29	114.54(19)
F1	C29	C28	119.33(19)
F1	C29	C30	117.4(2)
C30	C29	C28	123.1(2)
F2	C30	C29	118.0(2)
F2	C30	C31	119.56(19)
C29	C30	C31	122.3(2)
N6	C31	C30	122.7(2)
N6	C31	C32	122.5(2)
C30	C31	C32	114.77(19)
F3	C32	C31	119.38(19)
F3	C32	C33	118.1(2)
C33	C32	C31	122.5(2)
F4	C33	C28	119.57(18)
F4	C33	C32	117.66(19)
C32	C33	C28	122.7(2)
C37	C36	C14	122.80(19)
C37	C36	C41	116.24(19)
C41	C36	C14	120.96(19)
F5	C37	C36	119.88(19)
F5	C37	C38	118.1(2)
C36	C37	C38	122.0(2)
F6	C38	C37	118.5(2)
F6	C38	C39	120.28(19)
C39	C38	C37	121.2(2)
C40	C39	C38	117.56(19)
F7	C40	C39	120.03(18)
F7	C40	C41	118.48(19)
C39	C40	C41	121.5(2)
F8	C41	C36	119.73(18)
F8	C41	C40	118.75(19)
C36	C41	C40	121.5(2)
O1	C43	C42	112.3(2)

Table 15: Torsion Angles in ° for **Compound 19**.

Atom	Atom	Atom	Atom	Angle/°
F1	C29	C30	F2	1.2(3)
F1	C29	C30	C31	176.84(19)
F2	C30	C31	N6	-2.6(3)
F2	C30	C31	C32	175.90(18)
F3	C32	C33	F4	1.7(3)
F3	C32	C33	C28	-175.80(19)
F5	C37	C38	F6	-1.9(3)
F5	C37	C38	C39	-179.5(2)
F6	C38	C39	C40	-176.8(2)
F7	C40	C41	F8	2.6(3)
F7	C40	C41	C36	-177.89(18)
F10	C24	C25	F9	-0.2(3)
F10	C24	C25	C20	177.3(2)
F11	C22	C23	N5	5.7(4)
F11	C22	C23	C24	-177.0(2)
F12	C21	C22	F11	-0.4(3)
F12	C21	C22	C23	-178.3(2)
N1	C1	C2	C3	1.5(3)
N1	C1	C19	C18	-2.5(3)
N1	C1	C19	C20	179.4(2)
N1	C4	C5	N2	-7.1(3)
N1	C4	C5	C6	154.0(3)
N2	C5	C6	C7	1.6(3)
N2	C8	C9	C10	11.2(3)
N2	C8	C9	C28	-172.4(2)
N3	C10	C11	C12	-1.8(3)
N3	C13	C14	C15	-0.5(4)
N3	C13	C14	C36	-178.19(19)
N4	C15	C16	C17	0.5(3)
N4	C18	C19	C1	-3.2(4)
N4	C18	C19	C20	174.8(2)
N5	C23	C24	F10	-0.3(3)
N5	C23	C24	C25	177.5(2)
N6	C31	C32	F3	-5.8(3)
N6	C31	C32	C33	176.2(2)
C1	N1	C4	C3	2.8(3)
C1	N1	C4	C5	-171.47(19)
C1	C2	C3	C4	0.1(3)
C1	C19	C20	C21	-58.4(3)
C1	C19	C20	C25	120.2(2)
C2	C1	C19	C18	171.3(2)
C2	C1	C19	C20	-6.8(4)
C2	C3	C4	N1	-1.7(3)
C2	C3	C4	C5	170.7(3)
C3	C4	C5	N2	-178.9(3)
C3	C4	C5	C6	-17.8(5)
C4	N1	C1	C2	-2.7(3)
C4	N1	C1	C19	172.7(2)
C4	C5	C6	C7	-160.7(3)
C5	N2	C8	C7	3.5(2)
C5	N2	C8	C9	-167.2(2)
C5	C6	C7	C8	0.6(3)
C6	C7	C8	N2	-2.5(3)
C6	C7	C8	C9	166.8(2)
C7	C8	C9	C10	-156.8(2)
C7	C8	C9	C28	19.6(4)
C8	N2	C5	C4	163.06(19)
C8	N2	C5	C6	-3.2(3)
C8	C9	C10	N3	8.5(4)

Atom	Atom	Atom	Atom	Angle/°
C8	C9	C10	C11	-168.9(2)
C8	C9	C28	C29	60.7(3)
C8	C9	C28	C33	-118.2(2)
C9	C10	C11	C12	175.9(2)
C9	C28	C29	F1	4.2(3)
C9	C28	C29	C30	179.2(2)
C9	C28	C33	F4	1.4(3)
C9	C28	C33	C32	178.8(2)
C10	N3	C13	C12	-1.6(2)
C10	N3	C13	C14	177.8(2)
C10	C9	C28	C29	-122.7(2)
C10	C9	C28	C33	58.4(3)
C10	C11	C12	C13	0.9(3)
C11	C12	C13	N3	0.4(2)
C11	C12	C13	C14	-179.0(2)
C12	C13	C14	C15	178.7(2)
C12	C13	C14	C36	1.0(3)
C13	N3	C10	C9	-175.7(2)
C13	N3	C10	C11	2.1(2)
C13	C14	C15	N4	-5.0(4)
C13	C14	C15	C16	174.0(2)
C13	C14	C36	C37	-84.8(3)
C13	C14	C36	C41	94.8(2)
C14	C15	C16	C17	-178.7(2)
C14	C36	C37	F5	-0.9(3)
C14	C36	C37	C38	179.7(2)
C14	C36	C41	F8	-0.9(3)
C14	C36	C41	C40	179.6(2)
C15	N4	C18	C17	0.0(2)
C15	N4	C18	C19	179.1(2)
C15	C14	C36	C37	97.3(3)
C15	C14	C36	C41	-83.1(3)
C15	C16	C17	C18	-0.4(3)
C16	C17	C18	N4	0.3(3)
C16	C17	C18	C19	-178.8(2)
C17	C18	C19	C1	175.7(2)
C17	C18	C19	C20	-6.3(3)
C18	N4	C15	C14	178.9(2)
C18	N4	C15	C16	-0.3(2)
C18	C19	C20	C21	123.4(2)
C18	C19	C20	C25	-57.9(3)
C19	C1	C2	C3	-172.9(3)
C19	C20	C21	F12	-3.5(3)
C19	C20	C21	C22	179.6(2)
C19	C20	C25	F9	-1.2(3)
C19	C20	C25	C24	-178.7(2)
C20	C21	C22	F11	176.6(2)
C20	C21	C22	C23	-1.4(4)
C21	C20	C25	F9	177.55(19)
C21	C20	C25	C24	0.0(3)
C21	C22	C23	N5	-176.4(2)
C21	C22	C23	C24	0.9(3)
C22	C23	C24	F10	-177.8(2)
C22	C23	C24	C25	0.0(3)
C23	C24	C25	F9	-178.0(2)
C23	C24	C25	C20	-0.5(4)
C25	C20	C21	F12	177.73(19)
C25	C20	C21	C22	0.9(3)
C26	N5	C23	C22	27.6(3)
C26	N5	C23	C24	-149.6(2)
C27	N5	C23	C22	-113.6(3)
C27	N5	C23	C24	69.2(3)
C28	C9	C10	N3	-167.9(2)

Atom	Atom	Atom	Atom	Angle/°
C28	C9	C10	C11	14.8(4)
C28	C29	C30	F2	-173.87(19)
C28	C29	C30	C31	1.8(3)
C29	C28	C33	F4	-177.58(17)
C29	C28	C33	C32	-0.2(3)
C29	C30	C31	N6	-178.1(2)
C29	C30	C31	C32	0.4(3)
C30	C31	C32	F3	175.77(18)
C30	C31	C32	C33	-2.3(3)
C31	C32	C33	F4	179.76(18)
C31	C32	C33	C28	2.3(3)
C33	C28	C29	F1	-176.80(18)
C33	C28	C29	C30	-1.8(3)
C34	N6	C31	C30	-41.8(4)
C34	N6	C31	C32	139.9(2)
C35	N6	C31	C30	137.4(2)
C35	N6	C31	C32	-40.9(4)
C36	C14	C15	N4	172.6(2)
C36	C14	C15	C16	-8.3(3)
C36	C37	C38	F6	177.5(2)
C36	C37	C38	C39	-0.1(4)
C37	C36	C41	F8	178.82(19)
C37	C36	C41	C40	-0.7(3)
C37	C38	C39	C40	0.8(3)
C38	C39	C40	F7	177.84(19)
C38	C39	C40	C41	-1.5(3)
C39	C40	C41	F8	-178.03(19)
C39	C40	C41	C36	1.5(3)
C41	C36	C37	F5	179.4(2)
C41	C36	C37	C38	0.0(3)

Table 16: Hydrogen Bond information for **Compound 19**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N1	H1	N4	0.79(3)	1.98(3)	2.643(3)	141(3)
N2	H2	O1	0.86(3)	2.04(3)	2.894(3)	170(2)
N3	H3	N4	0.87(3)	2.32(3)	2.906(3)	125(2)
O1	H1A	N4	0.84	2.33	3.037(3)	142.0

Compound 20

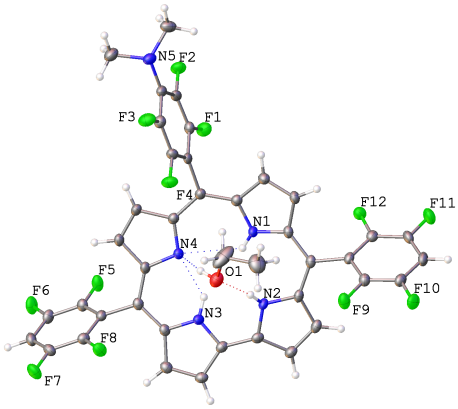
Report created with ReportPlus

Submitted by: **Léo Bucher**

Solved by: **Yoann Rousselin**

Sample ID: **20181025LB060**

Crystal Data and Experimental



Experimental. Single clear dark violet plate-shaped crystals of **Compound 20** were recrystallized from ethanol by slow evaporation. A suitable crystal 0.42 mm x 0.22 mm x 0.09 mm was selected and mounted on a MITIGEN holder oil on a Bruker D8 VENTURE diffractometer. The crystal was kept at a steady T = 100(1) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using the Intrinsic Phasing solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2018/3 of **ShelXL** (Sheldrick, 2015) using Least Squares minimization.

Crystal Data. $C_{41}H_{25}F_{12}N_5O$, M_r = 831.66, monoclinic, $C2/c$ (No. 15), a = 36.020(2) Å, b = 7.8480(5) Å, c = 27.7092(17) Å, β = 116.811(3)°, α = γ = 90°, V = 6990.8(8) Å^3, T = 100(1) K, Z = 8, Z' = 1, μ(CuK$_\alpha$) = 1.241, 28352 reflections measured, 6198 unique (R_{int} = 0.0419) which were used in all calculations. The final wR_2 was 0.1008 (all data) and R_1 was 0.0417 (I > 2(I)).

Compound	**20**
CCDC	**1910518**
Formula	$C_{41}H_{25}F_{12}N_5O$
$D_{calc.}$/ g cm^{-3}	1.580
μ/mm^{-1}	1.241
Formula Weight	831.66
Colour	clear dark violet
Shape	plate
Size/mm^3	0.42x0.22x0.09
T/K	100(1)
Crystal System	monoclinic
Space Group	$C2/c$
a/Å	36.020(2)
b/Å	7.8480(5)
c/Å	27.7092(17)
α/°	90
β/°	116.811(3)
γ/°	90
V/Å^3	6990.8(8)
Z	8
Z'	1
Wavelength/Å	1.54178
Radiation type	CuK$_\alpha$
Θ_{min}/°	2.749
Θ_{max}/°	66.805
Measured Refl.	28352
Independent Refl.	6198
Reflections with I > 2(I)	5377
R_{int}	0.0419
Parameters	545
Restraints	0
Largest Peak	0.361
Deepest Hole	-0.280
GooF	1.061
wR_2 (all data)	0.1008
wR_2	0.0967
R_1 (all data)	0.0497
R_1	0.0417

Structure Quality Indicators

Reflections:	d min (Cu) 0.84	I/σ 31.5	Rint 4.19%	complete 100%
Refinement:	Shift 0.000	Max Peak 0.4	Min Peak -0.3	GooF 1.061

A clear dark violet plate-shaped crystal with dimensions 0.42 mm x 0.22 mm x 0.09 mm was mounted on a MITIGEN holder oil. Data were collected using an Bruker D8 VENTURE diffractometer equipped with an Oxford Cryosystems low-temperature device operating at T = 100(1) K. Data were measured using ϕ and ω scans using CuK_α radiation. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) The maximum resolution that was achieved was Θ = 66.805° (0.84 Å). The diffraction pattern was indexed. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) and the unit cell was refined using **SAINT** (Bruker, V8.38A, after 2013) on 9845 reflections, 35% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.38A, after 2013). The final completeness is 99.80 % out to 66.805° in Θ. A multi-scan absorption correction was performed using **SADABS**-2016/2 (Bruker,2016) was used for absorption correction. wR_2(int) was 0.0911 before and 0.0613 after correction. The Ratio of minimum to maximum transmission is 0.8137. The absorption coefficient μ of this material is 1.241 mm^{-1} at this wavelength (λ = 1.542Å) and the minimum and maximum transmissions are 0.665 and 0.817. The structure was solved and the space group $C2/c$ (# 15) determined by the **ShelXT** (Sheldrick, 2015) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model, excepted those located on nitrogen atoms which were located in Fourier difference map. There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 8 and Z' is 1.

Table 17: Bond Lengths in Å for **Compound 20**.

Atom	Atom	Length/Å
F1	C21	1.343(2)
F2	C22	1.351(2)
F3	C24	1.347(2)
F4	C25	1.348(2)
F5	C35	1.345(2)
F6	C36	1.348(2)
F7	C38	1.344(2)
F8	C39	1.342(2)
F9	C33	1.342(2)
F10	C32	1.347(2)
F11	C30	1.345(2)
F12	C29	1.344(2)
N1	C1	1.373(3)
N1	C4	1.384(2)
C41	O1	1.423(3)
C41	C40	1.439(4)
N2	C6	1.372(3)
N2	C9	1.381(3)
N3	C10	1.357(3)
N3	C13	1.355(3)
N4	C15	1.387(2)
N4	C18	1.367(2)
N5	C23	1.414(3)
N5	C26	1.466(3)
N5	C27	1.460(3)
C1	C2	1.429(3)
C1	C19	1.399(3)

Atom	Atom	Length/Å
C2	C3	1.362(3)
C3	C4	1.424(3)
C4	C5	1.404(3)
C5	C6	1.413(3)
C5	C28	1.488(3)
C6	C7	1.410(3)
C7	C8	1.384(3)
C8	C9	1.401(3)
C9	C10	1.412(3)
C10	C11	1.415(3)
C11	C12	1.381(3)
C12	C13	1.424(3)
C13	C14	1.406(3)
C14	C15	1.412(3)
C14	C34	1.491(3)
C15	C16	1.439(3)
C16	C17	1.348(3)
C17	C18	1.444(3)
C18	C19	1.417(3)
C19	C20	1.497(3)
C20	C21	1.385(3)
C20	C25	1.385(3)
C21	C22	1.384(3)
C22	C23	1.387(3)
C23	C24	1.393(3)
C24	C25	1.378(3)
C28	C29	1.390(3)

Atom	Atom	Length/Å
C28	C33	1.398(3)
C29	C30	1.380(3)
C30	C31	1.374(3)
C31	C32	1.372(3)
C32	C33	1.378(3)
C34	C35	1.389(3)
C34	C39	1.391(3)
C35	C36	1.380(3)
C36	C37	1.378(3)
C37	C38	1.375(3)
C38	C39	1.378(3)

Table 18: Bond Angles in ° for **Compound 20**.

Atom	Atom	Atom	Angle/°
C1	N1	C4	111.82(16)
O1	C41	C40	112.3(2)
C6	N2	C9	110.40(16)
C13	N3	C10	112.28(17)
C18	N4	C15	106.30(15)
C23	N5	C26	117.13(18)
C23	N5	C27	113.90(16)
C27	N5	C26	112.47(17)
N1	C1	C2	105.45(16)
N1	C1	C19	125.19(18)
C19	C1	C2	129.08(18)
C3	C2	C1	108.50(17)
C2	C3	C4	109.19(17)
N1	C4	C3	104.92(16)
N1	C4	C5	124.87(18)
C5	C4	C3	130.07(18)
C4	C5	C6	123.32(17)
C4	C5	C28	120.55(17)
C6	C5	C28	116.12(17)
N2	C6	C5	120.76(17)
N2	C6	C7	106.29(17)
C7	C6	C5	132.76(18)
C8	C7	C6	108.59(17)
C7	C8	C9	107.73(17)
N2	C9	C8	106.98(17)
N2	C9	C10	114.92(17)
C8	C9	C10	137.41(18)
N3	C10	C9	115.37(17)
N3	C10	C11	106.29(17)
C9	C10	C11	138.32(18)
C12	C11	C10	107.68(17)
C11	C12	C13	108.05(17)
N3	C13	C12	105.67(17)
N3	C13	C14	118.22(18)
C14	C13	C12	136.02(18)
C13	C14	C15	122.67(18)
C13	C14	C34	117.88(17)
C15	C14	C34	119.44(17)
N4	C15	C14	124.76(17)
N4	C15	C16	109.20(17)
C14	C15	C16	125.89(18)
C17	C16	C15	107.57(17)
C16	C17	C18	106.98(17)
N4	C18	C17	109.96(17)
N4	C18	C19	125.62(17)
C19	C18	C17	124.39(17)
C1	C19	C18	127.24(18)
C1	C19	C20	116.72(17)
C18	C19	C20	115.76(16)
C21	C20	C19	123.88(18)
C21	C20	C25	115.10(17)
C25	C20	C19	120.98(18)
F1	C21	C20	119.53(17)
F1	C21	C22	117.88(18)
C22	C21	C20	122.58(19)
F2	C22	C21	117.38(19)
F2	C22	C23	120.36(18)
C21	C22	C23	122.25(19)
C22	C23	N5	126.31(19)
C22	C23	C24	115.04(18)
C24	C23	N5	118.62(19)
F3	C24	C23	119.32(17)
F3	C24	C25	118.30(18)
C25	C24	C23	122.35(19)
F4	C25	C20	119.51(17)
F4	C25	C24	117.86(18)
C24	C25	C20	122.61(19)
C29	C28	C5	124.09(18)
C29	C28	C33	115.84(18)
C33	C28	C5	119.89(19)
F12	C29	C28	120.22(17)
F12	C29	C30	118.03(19)
C30	C29	C28	121.74(19)
F11	C30	C29	118.7(2)
F11	C30	C31	119.81(18)
C31	C30	C29	121.5(2)
C32	C31	C30	117.56(19)
F10	C32	C31	120.44(18)
F10	C32	C33	118.08(19)
C31	C32	C33	121.5(2)
F9	C33	C28	120.15(17)
F9	C33	C32	118.06(19)
C32	C33	C28	121.8(2)
C35	C34	C14	122.97(18)
C35	C34	C39	115.87(18)
C39	C34	C14	121.15(18)
F5	C35	C34	119.80(17)
F5	C35	C36	118.43(18)
C36	C35	C34	121.77(19)
F6	C36	C35	118.57(19)
F6	C36	C37	119.78(18)
C37	C36	C35	121.65(19)
C38	C37	C36	117.17(19)
F7	C38	C37	120.57(18)
F7	C38	C39	117.99(19)
C37	C38	C39	121.4(2)
F8	C39	C34	119.70(17)
F8	C39	C38	118.18(19)
C38	C39	C34	122.10(19)

Table 19: Torsion Angles in ° for **Compound 20**.

Atom	Atom	Atom	Atom	Angle/°
F1	C21	C22	F2	1.1(3)
F1	C21	C22	C23	-177.92(17)
F2	C22	C23	N5	-3.5(3)
F2	C22	C23	C24	178.45(17)
F3	C24	C25	F4	1.9(3)
F3	C24	C25	C20	-176.68(18)
F5	C35	C36	F6	-0.8(3)
F5	C35	C36	C37	179.20(18)
F6	C36	C37	C38	-179.73(18)
F7	C38	C39	F8	0.1(3)
F7	C38	C39	C34	-178.45(18)
F10	C32	C33	F9	-0.2(3)
F10	C32	C33	C28	179.13(17)
F11	C30	C31	C32	-179.06(18)
F12	C29	C30	F11	-1.9(3)
F12	C29	C30	C31	178.63(18)
N1	C1	C2	C3	-1.9(2)
N1	C1	C19	C18	4.4(3)
N1	C1	C19	C20	178.02(18)
N1	C4	C5	C6	-7.2(3)
N1	C4	C5	C28	174.22(19)
N2	C6	C7	C8	0.9(2)
N2	C9	C10	N3	10.1(3)
N2	C9	C10	C11	-168.3(2)
N3	C10	C11	C12	0.4(2)
N3	C13	C14	C15	-2.0(3)
N3	C13	C14	C34	178.34(18)
N4	C15	C16	C17	-0.7(2)
N4	C18	C19	C1	3.4(3)
N4	C18	C19	C20	-170.20(19)
N5	C23	C24	F3	0.3(3)
N5	C23	C24	C25	-177.61(18)
C1	N1	C4	C3	-3.6(2)
C1	N1	C4	C5	172.48(19)
C1	C2	C3	C4	-0.2(2)
C1	C19	C20	C21	80.9(2)
C1	C19	C20	C25	-101.3(2)
C2	C1	C19	C18	-168.6(2)
C2	C1	C19	C20	5.0(3)
C2	C3	C4	N1	2.3(2)
C2	C3	C4	C5	-173.5(2)
C3	C4	C5	C6	167.8(2)
C3	C4	C5	C28	-10.8(3)
C4	N1	C1	C2	3.4(2)
C4	N1	C1	C19	-170.96(19)
C4	C5	C6	N2	-14.9(3)
C4	C5	C6	C7	159.3(2)
C4	C5	C28	C29	-60.0(3)
C4	C5	C28	C33	124.9(2)
C5	C6	C7	C8	-174.0(2)
C5	C28	C29	F12	6.9(3)
C5	C28	C29	C30	-171.82(18)
C5	C28	C33	F9	-7.4(3)
C5	C28	C33	C32	173.30(18)
C6	N2	C9	C8	1.2(2)
C6	N2	C9	C10	-171.01(17)
C6	C5	C28	C29	121.3(2)
C6	C5	C28	C33	-53.8(3)
C6	C7	C8	C9	-0.2(2)
C7	C8	C9	N2	-0.6(2)
C7	C8	C9	C10	168.9(2)

Atom	Atom	Atom	Atom	Angle/°
C8	C9	C10	N3	-158.8(2)
C8	C9	C10	C11	22.8(4)
C9	N2	C6	C5	174.32(18)
C9	N2	C6	C7	-1.3(2)
C9	C10	C11	C12	178.9(2)
C10	N3	C13	C12	1.8(2)
C10	N3	C13	C14	-175.39(18)
C10	C11	C12	C13	0.7(2)
C11	C12	C13	N3	-1.5(2)
C11	C12	C13	C14	175.0(2)
C12	C13	C14	C15	-178.1(2)
C12	C13	C14	C34	2.2(4)
C13	N3	C10	C9	179.65(17)
C13	N3	C10	C11	-1.5(2)
C13	C14	C15	N4	0.8(3)
C13	C14	C15	C16	-174.2(2)
C13	C14	C34	C35	-116.2(2)
C13	C14	C34	C39	62.6(3)
C14	C15	C16	C17	175.1(2)
C14	C34	C35	F5	-0.3(3)
C14	C34	C35	C36	179.06(18)
C14	C34	C39	F8	2.1(3)
C14	C34	C39	C38	-179.31(18)
C15	N4	C18	C17	0.0(2)
C15	N4	C18	C19	177.98(19)
C15	C14	C34	C35	64.2(3)
C15	C14	C34	C39	-117.1(2)
C15	C16	C17	C18	0.6(2)
C16	C17	C18	N4	-0.4(2)
C16	C17	C18	C19	-178.4(2)
C17	C18	C19	C1	-178.9(2)
C17	C18	C19	C20	7.5(3)
C18	N4	C15	C14	-175.41(19)
C18	N4	C15	C16	0.4(2)
C18	C19	C20	C21	-104.7(2)
C18	C19	C20	C25	73.0(2)
C19	C1	C2	C3	172.2(2)
C19	C20	C21	F1	-2.2(3)
C19	C20	C21	C22	177.11(18)
C19	C20	C25	F4	2.4(3)
C19	C20	C25	C24	-179.11(18)
C20	C21	C22	F2	-178.24(17)
C20	C21	C22	C23	2.7(3)
C21	C20	C25	F4	-179.69(17)
C21	C20	C25	C24	-1.2(3)
C21	C22	C23	N5	175.53(19)
C21	C22	C23	C24	-2.6(3)
C22	C23	C24	F3	178.54(18)
C22	C23	C24	C25	0.6(3)
C23	C24	C25	F4	179.79(18)
C23	C24	C25	C20	1.2(3)
C25	C20	C21	F1	179.91(17)
C25	C20	C21	C22	-0.8(3)
C26	N5	C23	C22	-32.6(3)
C26	N5	C23	C24	145.47(19)
C27	N5	C23	C22	101.6(2)
C27	N5	C23	C24	-80.4(2)
C28	C5	C6	N2	163.71(18)
C28	C5	C6	C7	-22.0(3)
C28	C29	C30	F11	176.82(18)
C28	C29	C30	C31	-2.7(3)
C29	C28	C33	F9	177.14(17)
C29	C28	C33	C32	-2.1(3)

Atom	Atom	Atom	Atom	Angle/°
C29	C30	C31	C32	0.4(3)
C30	C31	C32	F10	-178.19(18)
C30	C31	C32	C33	0.9(3)
C31	C32	C33	F9	-179.25(18)
C31	C32	C33	C28	0.1(3)
C33	C28	C29	F12	-177.91(16)
C33	C28	C29	C30	3.4(3)
C34	C14	C15	N4	-179.49(18)
C34	C14	C15	C16	5.4(3)
C34	C35	C36	F6	179.84(17)
C34	C35	C36	C37	-0.2(3)
C35	C34	C39	F8	-179.03(17)
C35	C34	C39	C38	-0.5(3)
C35	C36	C37	C38	0.3(3)
C36	C37	C38	F7	178.55(18)
C36	C37	C38	C39	-0.5(3)
C37	C38	C39	F8	179.21(18)
C37	C38	C39	C34	0.6(3)
C39	C34	C35	F5	-179.11(17)
C39	C34	C35	C36	0.2(3)

Table 20: Hydrogen Bond information for **Compound 20**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N1	H1	N4	0.83(2)	2.43(2)	2.959(2)	122.3(19)
N2	H2	O1	0.85(2)	2.07(2)	2.905(2)	172(2)
N3	H3	N4	0.87(2)	1.91(2)	2.610(2)	137(2)
O1	H1A	N4	0.84	2.25	3.020(2)	152.2

Compound 21

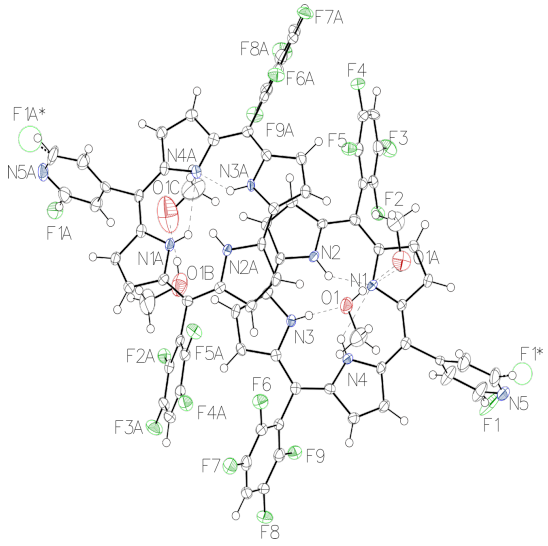
Report created with **ReportPlus**

Submitted by: **Léo Bucher**

Solved by: **Yoann Rousselin**

Sample ID: **20180925LB52twin**

Crystal Data and Experimental



Experimental. Single clear dark violet prism-shaped crystals of **Compound 21** were recrystallized from a mixture of methanol and heptane by slow evaporation. A suitable crystal 0.23 mm x 0.15 mm x 0.08 mm was selected and mounted on a MITIGEN holder oil on a Bruker D8 VENTURE diffractometer. The crystal was kept at a steady T = 100(1) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using the Intrinsic Phasing solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2018/3 of **ShelXL** (Sheldrick, 2015) using Least Squares minimization.

Crystal Data. $C_{38}H_{24}F_9N_5O_2$, M_r = 753.62, triclinic, P-1 (No. 2), a = 7.3448(2) Å, b = 15.9784(5) Å, c = 28.5025(9) Å, α = 104.448(2)°, β = 91.342(2)°, γ = 93.085(2)°, V = 3232.17(17) Å^3, T = 100(1) K, Z = 4, Z' = 2, μ(CuK$_\alpha$) = 1.162, 17364 reflections measured, 17364 unique (R_{int} = .) which were used in all calculations. The final wR_2 was 0.1357 (all data) and R_1 was 0.0681 (I > 2(I)).

Compound	**21**
CCDC	**1910519**
Formula	$C_{38}H_{24}F_9N_5O_2$
$D_{calc.}$/ g cm^{-3}	1.549
μ/mm^{-1}	1.162
Formula Weight	753.62
Colour	clear dark violet
Shape	prism
Size/mm^3	0.23x0.15x0.08
T/K	100(1)
Crystal System	triclinic
Space Group	P-1
a/Å	7.3448(2)
b/Å	15.9784(5)
c/Å	28.5025(9)
α/°	104.448(2)
β/°	91.342(2)
γ/°	93.085(2)
V/Å^3	3232.17(17)
Z	4
Z'	2
Wavelength/Å	1.54178
Radiation type	CuK$_\alpha$
Θ_{min}/°	2.861
Θ_{max}/°	66.718
Measured Refl.	17364
Independent Refl.	17364
Reflections with I > 2(I)	13612
R_{int}	.
Parameters	1006
Restraints	50
Largest Peak	0.866
Deepest Hole	-0.489
GooF	1.068
wR_2 (all data)	0.1357
wR_2	0.1248
R_1 (all data)	0.0925
R_1	0.0681

Structure Quality Indicators

Reflections:	d min (Cu) 0.84	I/σ 17.8	Rint Merged!	complete 97%
Refinement:	Shift 0.000	Max Peak 0.9	Min Peak -0.5	GooF 1.068

A clear dark violet prism-shaped crystal with dimensions 0.23 mm x 0.15 mm x 0.08 mm was mounted on a MITIGEN holder oil. Data were collected using a Bruker D8 VENTURE diffractometer equipped with an Oxford Cryosystems low-temperature device operating at T = 100(1) K. Data were measured using ϕ and ω scans using CuK$_\alpha$ radiation. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) The maximum resolution that was achieved was Θ = 66.718° (0.84 Å). The diffraction pattern was indexed. The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker, 2015) and the unit cell was refined using **SAINT** (Bruker, V8.38A, after 2013) on 5136 reflections, 30% of the observed reflections. Data reduction, scaling and absorption corrections were performed using **SAINT** (Bruker, V8.38A, after 2013). The final completeness is 94.50 % out to 66.718° in Θ. A multi-scan absorption correction was performed using TWINABS-2012/1 (Bruker,2012) was used for absorption correction. Final HKLF 4 output contains 43905 reflections, R_{int} = 0.0656 (25067 with I > 3sig(I), R_{int} = 0.0505). The absorption coefficient μ of this material is 1.162 mm^{-1} at this wavelength (λ = 1.542Å) and the minimum and maximum transmissions are 0.790 and 0.860. The structure was solved and the space group P-1 (# 2) determined by the **ShelXT** (Sheldrick, 2015) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically, excepted minor disordered fluorine atom F1* and F1A* (72.2%/27.8%). Hydrogen atom positions were calculated geometrically and refined using the riding model, excepted those located on nitrogen atoms which were located in Fourier difference map. The value of Z' is 2. This means that there are two independent molecules in the asymmetric unit. Several crystals examined proved to have multiple domains. The final data crystal, while still a multiple, could be described having primarily two domains and was treated as such. Orientation matrices for the two domains were determined using the program **CELL_NOW** (Bruker, 2008) and the data were processed further using **TWINABS** (Bruker, 2008). HKLF 5 was employed, BASF specifies the fractional volume contributions of the various twin components. The crystal was refined as a non-merohedral twin with a minor twin component of 0.452(1).

Table 21: Bond Lengths in Å for **Compound 21**.

Atom	Atom	Length/Å
F1	C29	1.298(7)
F1*	C28	1.198(13)
F2	C25	1.348(5)
F3	C24	1.346(6)
F4	C22	1.351(5)
F5	C21	1.347(5)
F6	C32	1.342(5)
F7	C33	1.347(5)
F8	C35	1.353(6)
F9	C36	1.351(5)
N1	C1	1.367(5)
N1	C4	1.384(5)
N2	C6	1.358(5)
N2	C9	1.369(5)
N3	C10	1.383(5)
N3	C13	1.375(5)
N4	C15	1.388(5)
N4	C18	1.379(5)
N5	C28	1.311(8)
N5	C29	1.296(7)
C1	C2	1.450(6)

Atom	Atom	Length/Å
C1	C19	1.409(6)
C2	C3	1.351(6)
C3	C4	1.439(6)
C4	C5	1.419(6)
C5	C6	1.407(6)
C5	C20	1.492(6)
C6	C7	1.424(5)
C7	C8	1.375(6)
C8	C9	1.415(6)
C9	C10	1.401(6)
C10	C11	1.410(6)
C11	C12	1.381(6)
C12	C13	1.409(6)
C13	C14	1.416(6)
C14	C15	1.398(6)
C14	C31	1.484(6)
C15	C16	1.422(6)
C16	C17	1.359(6)
C17	C18	1.422(6)
C18	C19	1.396(6)
C19	C26	1.509(6)

Atom	Atom	Length/Å
C20	C21	1.387(6)
C20	C25	1.389(6)
C21	C22	1.379(6)
C22	C23	1.363(7)
C23	C24	1.383(7)
C24	C25	1.378(6)
C26	C27	1.382(7)
C26	C30	1.360(7)
C27	C28	1.367(7)
C29	C30	1.374(7)
C31	C32	1.388(6)
C31	C36	1.391(6)
C32	C33	1.379(6)
C33	C34	1.373(7)
C34	C35	1.373(7)
C35	C36	1.386(6)
F1A	C29A	1.301(7)
F1A*	C28A	1.142(17)
F2A	C25A	1.345(5)
F3A	C24A	1.348(5)
F4A	C22A	1.349(5)
F5A	C21A	1.349(5)
F6A	C32A	1.346(5)
F7A	C33A	1.354(5)
F8A	C35A	1.351(6)
F9A	C36A	1.352(5)
N1A	C1A	1.376(5)
N1A	C4A	1.381(5)
N2A	C6A	1.375(5)
N2A	C9A	1.374(5)
N3A	C10A	1.359(5)
N3A	C13A	1.361(5)
O1C	C37C	1.384(8)
N4A	C15A	1.383(5)
N4A	C18A	1.373(5)
N5A	C28A	1.340(7)
N5A	C29A	1.286(7)
C1A	C2A	1.429(6)
C1A	C19A	1.400(6)

Atom	Atom	Length/Å
C2A	C3A	1.361(6)
C3A	C4A	1.419(6)
C4A	C5A	1.412(6)
C5A	C6A	1.408(6)
C5A	C20A	1.482(6)
C6A	C7A	1.417(6)
C7A	C8A	1.386(6)
C8A	C9A	1.404(6)
C9A	C10A	1.414(6)
C10A	C11A	1.412(6)
C11A	C12A	1.376(6)
C12A	C13A	1.420(6)
C13A	C14A	1.401(6)
C14A	C15A	1.419(6)
C14A	C31A	1.496(6)
C15A	C16A	1.438(6)
C16A	C17A	1.350(6)
C17A	C18A	1.441(6)
C18A	C19A	1.411(6)
C19A	C26A	1.498(5)
C20A	C21A	1.393(6)
C20A	C25A	1.387(6)
C21A	C22A	1.373(6)
C22A	C23A	1.372(7)
C23A	C24A	1.364(7)
C24A	C25A	1.385(6)
C26A	C27A	1.381(7)
C26A	C30A	1.381(7)
C27A	C28A	1.380(7)
C29A	C30A	1.385(6)
C31A	C32A	1.389(6)
C31A	C36A	1.376(6)
C32A	C33A	1.385(6)
C33A	C34A	1.373(7)
C34A	C35A	1.366(7)
C35A	C36A	1.383(6)
O1	C37	1.420(6)
O1A	C37A	1.422(6)
O1B	C37B	1.463(7)

Table 22: Bond Angles in ° for **Compound 21**.

Atom	Atom	Atom	Angle/°
C1	N1	C4	106.6(3)
C6	N2	C9	111.8(3)
C13	N3	C10	109.8(3)
C18	N4	C15	111.5(3)
C29	N5	C28	113.3(5)
N1	C1	C2	109.7(3)
N1	C1	C19	125.2(4)
C19	C1	C2	125.2(4)
C3	C2	C1	106.9(4)
C2	C3	C4	107.5(4)
N1	C4	C3	109.4(4)
N1	C4	C5	124.0(4)
C5	C4	C3	126.6(4)
C4	C5	C20	119.5(4)
C6	C5	C4	122.7(4)
C6	C5	C20	117.7(4)
N2	C6	C5	119.4(4)

Atom	Atom	Atom	Angle/°
N2	C6	C7	106.0(3)
C5	C6	C7	134.2(4)
C8	C7	C6	107.9(4)
C7	C8	C9	108.3(4)
N2	C9	C8	105.8(4)
N2	C9	C10	116.9(4)
C10	C9	C8	136.7(4)
N3	C10	C9	116.2(4)
N3	C10	C11	107.1(4)
C9	C10	C11	134.5(4)
C12	C11	C10	107.7(4)
C11	C12	C13	108.5(4)
N3	C13	C12	106.9(4)
N3	C13	C14	120.4(4)
C12	C13	C14	131.9(4)
C13	C14	C31	118.5(4)
C15	C14	C13	122.6(4)

Atom	Atom	Atom	Angle/°
C15	C14	C31	118.8(4)
N4	C15	C14	125.7(4)
N4	C15	C16	105.1(4)
C14	C15	C16	129.2(4)
C17	C16	C15	109.0(4)
C16	C17	C18	109.1(4)
N4	C18	C17	105.3(4)
N4	C18	C19	124.9(4)
C19	C18	C17	129.8(4)
C1	C19	C26	117.8(4)
C18	C19	C1	127.1(4)
C18	C19	C26	115.1(4)
C21	C20	C5	121.2(4)
C21	C20	C25	116.1(4)
C25	C20	C5	122.6(4)
F5	C21	C20	120.3(4)
F5	C21	C22	117.8(4)
C22	C21	C20	121.9(4)
F4	C22	C21	118.7(4)
F4	C22	C23	119.9(4)
C23	C22	C21	121.4(4)
C22	C23	C24	117.7(4)
F3	C24	C23	120.3(4)
F3	C24	C25	118.7(4)
C25	C24	C23	121.0(5)
F2	C25	C20	120.3(4)
F2	C25	C24	117.8(4)
C24	C25	C20	121.9(4)
C27	C26	C19	122.0(4)
C30	C26	C19	120.4(4)
C30	C26	C27	117.5(4)
C28	C27	C26	117.7(6)
F1*	C28	N5	101.7(8)
F1*	C28	C27	131.1(9)
N5	C28	C27	126.2(6)
F1	C29	C30	120.6(6)
N5	C29	F1	111.8(5)
N5	C29	C30	127.3(6)
C26	C30	C29	117.6(5)
C32	C31	C14	121.6(4)
C32	C31	C36	115.9(4)
C36	C31	C14	122.4(4)
F6	C32	C31	120.0(4)
F6	C32	C33	118.2(4)
C33	C32	C31	121.8(4)
F7	C33	C32	118.7(5)
F7	C33	C34	119.7(4)
C34	C33	C32	121.6(5)
C35	C34	C33	117.6(4)
F8	C35	C34	120.3(4)
F8	C35	C36	118.6(5)
C34	C35	C36	121.1(5)
F9	C36	C31	120.4(4)
F9	C36	C35	117.7(4)
C35	C36	C31	121.9(5)
C1A	N1A	C4A	110.8(3)
C9A	N2A	C6A	110.8(3)
C10A	N3A	C13A	111.8(3)
C18A	N4A	C15A	106.8(3)
C29A	N5A	C28A	114.2(4)
N1A	C1A	C2A	105.9(4)
N1A	C1A	C19A	125.1(4)
C19A	C1A	C2A	129.0(4)

Atom	Atom	Atom	Angle/°
C3A	C2A	C1A	108.4(4)
C2A	C3A	C4A	108.8(4)
N1A	C4A	C3A	106.0(3)
N1A	C4A	C5A	124.7(4)
C5A	C4A	C3A	129.2(4)
C4A	C5A	C20A	119.3(4)
C6A	C5A	C4A	123.2(4)
C6A	C5A	C20A	117.4(4)
N2A	C6A	C5A	120.9(4)
N2A	C6A	C7A	106.2(4)
C5A	C6A	C7A	132.1(4)
C8A	C7A	C6A	108.1(4)
C7A	C8A	C9A	108.1(4)
N2A	C9A	C8A	106.8(4)
N2A	C9A	C10A	116.3(4)
C8A	C9A	C10A	135.0(4)
N3A	C10A	C9A	116.8(4)
N3A	C10A	C11A	106.4(4)
C11A	C10A	C9A	136.2(4)
C12A	C11A	C10A	107.8(4)
C11A	C12A	C13A	108.2(4)
N3A	C13A	C12A	105.6(4)
N3A	C13A	C14A	119.4(4)
C14A	C13A	C12A	134.3(4)
C13A	C14A	C15A	122.5(4)
C13A	C14A	C31A	118.6(4)
C15A	C14A	C31A	118.8(4)
N4A	C15A	C14A	124.6(4)
N4A	C15A	C16A	109.2(4)
C14A	C15A	C16A	126.2(4)
C17A	C16A	C15A	107.2(4)
C16A	C17A	C18A	107.6(4)
N4A	C18A	C17A	109.1(4)
N4A	C18A	C19A	125.5(4)
C19A	C18A	C17A	125.4(4)
C1A	C19A	C18A	126.5(4)
C1A	C19A	C26A	115.9(4)
C18A	C19A	C26A	117.6(4)
C21A	C20A	C5A	121.1(4)
C25A	C20A	C5A	123.2(4)
C25A	C20A	C21A	115.6(4)
F5A	C21A	C20A	119.8(4)
F5A	C21A	C22A	117.8(4)
C22A	C21A	C20A	122.4(4)
F4A	C22A	C21A	118.5(4)
F4A	C22A	C23A	120.4(4)
C23A	C22A	C21A	121.1(4)
C24A	C23A	C22A	117.7(4)
F3A	C24A	C23A	119.8(4)
F3A	C24A	C25A	118.5(4)
C23A	C24A	C25A	121.7(4)
F2A	C25A	C20A	120.5(4)
F2A	C25A	C24A	117.9(4)
C24A	C25A	C20A	121.6(4)
C27A	C26A	C19A	122.2(4)
C30A	C26A	C19A	120.1(4)
C30A	C26A	C27A	117.7(4)
C28A	C27A	C26A	118.5(5)
F1A*	C28A	N5A	106.9(10)
F1A*	C28A	C27A	127.7(11)
N5A	C28A	C27A	124.8(5)
F1A	C29A	C30A	119.6(6)
N5A	C29A	F1A	112.8(5)

Atom	Atom	Atom	Angle/°
N5A	C29A	C30A	127.5(5)
C26A	C30A	C29A	117.2(5)
C32A	C31A	C14A	121.1(4)
C36A	C31A	C14A	122.8(4)
C36A	C31A	C32A	116.1(4)
F6A	C32A	C31A	120.2(4)
F6A	C32A	C33A	118.2(4)
C33A	C32A	C31A	121.6(4)
F7A	C33A	C32A	118.2(4)

Atom	Atom	Atom	Angle/°
F7A	C33A	C34A	120.1(4)
C34A	C33A	C32A	121.7(5)
C35A	C34A	C33A	116.8(4)
F8A	C35A	C34A	119.5(4)
F8A	C35A	C36A	118.4(5)
C34A	C35A	C36A	122.1(5)
F9A	C36A	C31A	120.5(4)
F9A	C36A	C35A	117.8(4)
C31A	C36A	C35A	121.8(4)

Table 23: Torsion Angles in ° for **Compound 21**.

Atom	Atom	Atom	Atom	Angle/°
F1	C29	C30	C26	-174.2(5)
F3	C24	C25	F2	-0.3(6)
F3	C24	C25	C20	-178.6(4)
F4	C22	C23	C24	-179.9(4)
F5	C21	C22	F4	-2.2(6)
F5	C21	C22	C23	178.0(4)
F6	C32	C33	F7	1.9(6)
F6	C32	C33	C34	-179.1(4)
F7	C33	C34	C35	-179.9(4)
F8	C35	C36	F9	0.6(6)
F8	C35	C36	C31	178.8(4)
N1	C1	C2	C3	-0.6(5)
N1	C1	C19	C18	0.8(7)
N1	C1	C19	C26	179.8(4)
N1	C4	C5	C6	5.0(7)
N1	C4	C5	C20	-170.3(4)
N2	C6	C7	C8	-2.8(5)
N2	C9	C10	N3	7.5(6)
N2	C9	C10	C11	-153.0(5)
N3	C10	C11	C12	-0.2(5)
N3	C13	C14	C15	-16.0(6)
N3	C13	C14	C31	167.1(4)
N4	C15	C16	C17	-1.0(5)
N4	C18	C19	C1	1.9(7)
N4	C18	C19	C26	-177.1(4)
N5	C29	C30	C26	-1.6(9)
C1	N1	C4	C3	-1.2(5)
C1	N1	C4	C5	-178.9(4)
C1	C2	C3	C4	-0.1(5)
C1	C19	C26	C27	92.7(5)
C1	C19	C26	C30	-88.6(5)
C2	C1	C19	C18	-179.5(4)
C2	C1	C19	C26	-0.4(6)
C2	C3	C4	N1	0.8(5)
C2	C3	C4	C5	178.5(4)
C3	C4	C5	C6	-172.4(4)
C3	C4	C5	C20	12.4(7)
C4	N1	C1	C2	1.1(5)
C4	N1	C1	C19	-179.1(4)
C4	C5	C6	N2	4.7(6)
C4	C5	C6	C7	-166.2(5)
C4	C5	C20	C21	-131.1(4)
C4	C5	C20	C25	53.5(6)
C5	C6	C7	C8	169.1(5)
C5	C20	C21	F5	6.6(6)
C5	C20	C21	C22	-175.1(4)
C5	C20	C25	F2	-3.0(6)

Atom	Atom	Atom	Atom	Angle/°
C5	C20	C25	C24	175.2(4)
C6	N2	C9	C8	-4.2(5)
C6	N2	C9	C10	168.5(4)
C6	C5	C20	C21	53.4(6)
C6	C5	C20	C25	-122.1(5)
C6	C7	C8	C9	0.3(5)
C7	C8	C9	N2	2.3(5)
C7	C8	C9	C10	-168.2(5)
C8	C9	C10	N3	177.2(5)
C8	C9	C10	C11	16.7(9)
C9	N2	C6	C5	-168.9(4)
C9	N2	C6	C7	4.4(5)
C9	C10	C11	C12	161.5(5)
C10	N3	C13	C12	-2.7(5)
C10	N3	C13	C14	168.3(4)
C10	C11	C12	C13	-1.4(5)
C11	C12	C13	N3	2.5(5)
C11	C12	C13	C14	-167.1(5)
C12	C13	C14	C15	152.4(5)
C12	C13	C14	C31	-24.5(7)
C13	N3	C10	C9	-163.7(4)
C13	N3	C10	C11	1.8(5)
C13	C14	C15	N4	-7.3(7)
C13	C14	C15	C16	171.7(4)
C13	C14	C31	C32	-57.1(6)
C13	C14	C31	C36	123.2(5)
C14	C15	C16	C17	179.9(4)
C14	C31	C32	F6	-1.3(6)
C14	C31	C32	C33	-179.2(4)
C14	C31	C36	F9	-2.1(6)
C14	C31	C36	C35	179.7(4)
C15	N4	C18	C17	0.9(5)
C15	N4	C18	C19	-177.6(4)
C15	C14	C31	C32	125.9(5)
C15	C14	C31	C36	-53.8(6)
C15	C16	C17	C18	1.5(5)
C16	C17	C18	N4	-1.5(5)
C16	C17	C18	C19	176.9(5)
C17	C18	C19	C1	-176.1(5)
C17	C18	C19	C26	4.8(7)
C18	N4	C15	C14	179.2(4)
C18	N4	C15	C16	0.0(5)
C18	C19	C26	C27	-88.2(5)
C18	C19	C26	C30	90.6(5)
C19	C1	C2	C3	179.6(4)
C19	C26	C27	C28	-177.4(4)
C19	C26	C30	C29	-178.4(4)
C20	C5	C6	N2	-179.9(4)
C20	C5	C6	C7	9.1(7)
C20	C21	C22	F4	179.5(4)
C20	C21	C22	C23	-0.4(7)
C21	C20	C25	F2	-178.7(4)
C21	C20	C25	C24	-0.4(6)
C21	C22	C23	C24	0.0(7)
C22	C23	C24	F3	178.8(4)
C22	C23	C24	C25	0.2(7)
C23	C24	C25	F2	178.3(4)
C23	C24	C25	C20	0.1(7)
C25	C20	C21	F5	-177.7(4)
C25	C20	C21	C22	0.6(6)
C26	C27	C28	F1*	158.1(9)
C26	C27	C28	N5	-8.1(9)
C27	C26	C30	C29	0.4(7)

Atom	Atom	Atom	Atom	Angle/°
C28	N5	C29	F1	171.4(5)
C28	N5	C29	C30	-1.9(8)
C29	N5	C28	F1*	-162.5(7)
C29	N5	C28	C27	6.8(8)
C30	C26	C27	C28	3.8(7)
C31	C14	C15	N4	169.6(4)
C31	C14	C15	C16	-11.4(7)
C31	C32	C33	F7	179.9(4)
C31	C32	C33	C34	-1.1(7)
C32	C31	C36	F9	178.2(4)
C32	C31	C36	C35	0.0(6)
C32	C33	C34	C35	1.1(7)
C33	C34	C35	F8	-179.3(4)
C33	C34	C35	C36	-0.5(7)
C34	C35	C36	F9	-178.2(4)
C34	C35	C36	C31	0.0(7)
C36	C31	C32	F6	178.5(4)
C36	C31	C32	C33	0.5(6)
F1A	C29A	C30A	C26A	179.4(4)
F3A	C24A	C25A	F2A	0.6(6)
F3A	C24A	C25A	C20A	-179.3(4)
F4A	C22A	C23A	C24A	178.9(4)
F5A	C21A	C22A	F4A	-2.2(6)
F5A	C21A	C22A	C23A	177.2(4)
F6A	C32A	C33A	F7A	1.3(6)
F6A	C32A	C33A	C34A	-177.9(4)
F7A	C33A	C34A	C35A	-179.3(4)
F8A	C35A	C36A	F9A	1.1(6)
F8A	C35A	C36A	C31A	-179.5(4)
N1A	C1A	C2A	C3A	-0.3(5)
N1A	C1A	C19A	C18A	-2.2(7)
N1A	C1A	C19A	C26A	178.4(4)
N1A	C4A	C5A	C6A	7.6(7)
N1A	C4A	C5A	C20A	-168.2(4)
N2A	C6A	C7A	C8A	-1.3(5)
N2A	C9A	C10A	N3A	-5.1(6)
N2A	C9A	C10A	C11A	-174.4(5)
N3A	C10A	C11A	C12A	-1.9(5)
N3A	C13A	C14A	C15A	-4.5(6)
N3A	C13A	C14A	C31A	175.5(4)
N4A	C15A	C16A	C17A	-0.7(5)
N4A	C18A	C19A	C1A	0.8(7)
N4A	C18A	C19A	C26A	-179.8(4)
N5A	C29A	C30A	C26A	-1.6(8)
C1A	N1A	C4A	C3A	-0.3(5)
C1A	N1A	C4A	C5A	-179.9(4)
C1A	C2A	C3A	C4A	0.1(5)
C1A	C19A	C26A	C27A	106.7(5)
C1A	C19A	C26A	C30A	-73.2(6)
C2A	C1A	C19A	C18A	174.6(5)
C2A	C1A	C19A	C26A	-4.8(7)
C2A	C3A	C4A	N1A	0.1(5)
C2A	C3A	C4A	C5A	179.7(4)
C3A	C4A	C5A	C6A	-171.9(4)
C3A	C4A	C5A	C20A	12.3(7)
C4A	N1A	C1A	C2A	0.3(5)
C4A	N1A	C1A	C19A	177.8(4)
C4A	C5A	C6A	N2A	13.9(6)
C4A	C5A	C6A	C7A	-154.3(5)
C4A	C5A	C20A	C21A	-132.4(4)
C4A	C5A	C20A	C25A	52.3(6)
C5A	C6A	C7A	C8A	168.2(4)
C5A	C20A	C21A	F5A	6.9(6)

Atom	Atom	Atom	Atom	Angle/°
C5A	C20A	C21A	C22A	-176.0(4)
C5A	C20A	C25A	F2A	-3.1(6)
C5A	C20A	C25A	C24A	176.7(4)
C6A	N2A	C9A	C8A	-2.6(5)
C6A	N2A	C9A	C10A	163.9(4)
C6A	C5A	C20A	C21A	51.6(6)
C6A	C5A	C20A	C25A	-123.8(4)
C6A	C7A	C8A	C9A	-0.3(5)
C7A	C8A	C9A	N2A	1.7(5)
C7A	C8A	C9A	C10A	-161.0(5)
C8A	C9A	C10A	N3A	156.5(5)
C8A	C9A	C10A	C11A	-12.9(9)
C9A	N2A	C6A	C5A	-168.5(4)
C9A	N2A	C6A	C7A	2.4(5)
C9A	C10A	C11A	C12A	168.2(5)
C10A	N3A	C13A	C12A	-3.7(5)
C10A	N3A	C13A	C14A	168.4(4)
C10A	C11A	C12A	C13A	-0.3(5)
C11A	C12A	C13A	N3A	2.3(5)
C11A	C12A	C13A	C14A	-168.0(5)
C12A	C13A	C14A	C15A	164.8(5)
C12A	C13A	C14A	C31A	-15.2(7)
C13A	N3A	C10A	C9A	-168.8(4)
C13A	N3A	C10A	C11A	3.5(5)
C13A	C14A	C15A	N4A	-5.9(7)
C13A	C14A	C15A	C16A	173.1(4)
C13A	C14A	C31A	C32A	-56.6(6)
C13A	C14A	C31A	C36A	123.9(5)
C14A	C15A	C16A	C17A	-179.8(4)
C14A	C31A	C32A	F6A	-1.0(6)
C14A	C31A	C32A	C33A	-178.6(4)
C14A	C31A	C36A	F9A	-2.5(6)
C14A	C31A	C36A	C35A	178.1(4)
C15A	N4A	C18A	C17A	0.1(5)
C15A	N4A	C18A	C19A	178.0(4)
C15A	C14A	C31A	C32A	123.4(4)
C15A	C14A	C31A	C36A	-56.1(6)
C15A	C16A	C17A	C18A	0.7(5)
C16A	C17A	C18A	N4A	-0.5(5)
C16A	C17A	C18A	C19A	-178.5(4)
C17A	C18A	C19A	C1A	178.4(5)
C17A	C18A	C19A	C26A	-2.2(7)
C18A	N4A	C15A	C14A	179.5(4)
C18A	N4A	C15A	C16A	0.3(5)
C18A	C19A	C26A	C27A	-72.8(6)
C18A	C19A	C26A	C30A	107.3(5)
C19A	C1A	C2A	C3A	-177.6(5)
C19A	C26A	C27A	C28A	-179.2(4)
C19A	C26A	C30A	C29A	180.0(4)
C20A	C5A	C6A	N2A	-170.2(4)
C20A	C5A	C6A	C7A	21.6(7)
C20A	C21A	C22A	F4A	-179.4(4)
C20A	C21A	C22A	C23A	0.0(7)
C21A	C20A	C25A	F2A	-178.7(4)
C21A	C20A	C25A	C24A	1.1(6)
C21A	C22A	C23A	C24A	-0.5(7)
C22A	C23A	C24A	F3A	178.9(4)
C22A	C23A	C24A	C25A	1.3(7)
C23A	C24A	C25A	F2A	178.1(4)
C23A	C24A	C25A	C20A	-1.7(7)
C25A	C20A	C21A	F5A	-177.4(4)
C25A	C20A	C21A	C22A	-0.3(6)
C26A	C27A	C28A	F1A*	170.2(12)

Atom	Atom	Atom	Atom	Angle/°
C26A	C27A	C28A	N5A	-0.2(8)
C27A	C26A	C30A	C29A	0.1(7)
C28A	N5A	C29A	F1A	-178.9(5)
C28A	N5A	C29A	C30A	2.0(8)
C29A	N5A	C28A	F1A*	-173.1(10)
C29A	N5A	C28A	C27A	-1.1(8)
C30A	C26A	C27A	C28A	0.6(7)
C31A	C14A	C15A	N4A	174.0(4)
C31A	C14A	C15A	C16A	-7.0(7)
C31A	C32A	C33A	F7A	179.1(4)
C31A	C32A	C33A	C34A	-0.2(7)
C32A	C31A	C36A	F9A	178.0(4)
C32A	C31A	C36A	C35A	-1.4(6)
C32A	C33A	C34A	C35A	0.0(7)
C33A	C34A	C35A	F8A	-179.7(4)
C33A	C34A	C35A	C36A	-0.5(7)
C34A	C35A	C36A	F9A	-178.1(4)
C34A	C35A	C36A	C31A	1.3(7)
C36A	C31A	C32A	F6A	178.6(4)
C36A	C31A	C32A	C33A	0.9(6)

Table 24: Hydrogen Bond information for **Compound 21**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N2	H2	N1	0.90(5)	1.91(5)	2.640(5)	136(4)
N3	H3	O1	0.89(4)	1.94(4)	2.828(5)	177(4)
N4	H4	N1	0.79(5)	2.36(5)	2.921(5)	129(4)
N1A	H1A	N4A	0.81(4)	2.39(5)	2.918(5)	124(4)
N2A	H2AA	O1B[1]	0.85(5)	2.00(5)	2.840(5)	166(4)
N3A	H3AA	N4A	0.85	2.04	2.644(5)	127.2
O1C	H1C	N4A[2]	0.84	2.49	3.184(8)	141.1
O1	H1	O1A	0.84	1.94	2.779(5)	173.5
O1A	H1AA	N1	0.84	2.33	3.110(5)	154.2
O1B	H1B	O1C	0.84	1.91	2.705(9)	157.8

[1]-1+x,+y,+z; [2]1+x,+y,+z

Table 25: Atomic Occupancies for all atoms that are not fully occupied in **Compound 21**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
F1	0.722(5)	H28	0.722(5)	F1A	0.722(5)	H28A	0.722(5)
F1*	0.278(5)	H29	0.278(5)	F1A*	0.278(5)	H29A	0.278(5)

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